U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-296 835

Analysis of Organic Air Pollutants by Gas Chromatography and Mass Spectroscopy

Research Triangle Inst, Research Triangle Park, NC

Prepared for

Environmental Sciences Research Lab, Research Triangle Park, NC

Mar 79

United States
Environmental Protection
Agency

Environmental Sciences Research
Laboratory
Research Triangle Park NC 27711

EPA-600/2-79-057
March 1979

Research and Development

PB 296835

EPA

Analysis of Organic Air Pollutants by Gas Chromatography and Mass Spectroscopy

Final Report

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

RESEARCH REPORTING SERIES

Research reports of the Office of Research and Development, U.S. Environmental Protection Agency, have been grouped into nine series. These nine broad categories were established to facilitate further development and application of environmental technology. Elimination of traditional grouping was consciously planned to foster technology transfer and a maximum interface in related fields. The nine series are:

1. Environmental Health Effects Research
2. Environmental Protection Technology
3. Ecological Research
4. Environmental Monitoring
5. Socioeconomic Environmental Studies
6. Scientific and Technical Assessment Reports (STAR)
7. Interagency Energy-Environment Research and Development
8. "Special" Reports
9. Miscellaneous Reports

This report has been assigned to the ENVIRONMENTAL PROTECTION TECHNOLOGY series. This series describes research performed to develop and demonstrate instrumentation, equipment, and methodology to repair or prevent environmental degradation from point and non-point sources of pollution. This work provides the new or improved technology required for the control and treatment of pollution sources to meet environmental quality standards.

This document is available to the public through the National Technical Information Service, Springfield, Virginia 22161.

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/2-79-057	2.	3. RECIPIENT'S ACCESSION NO. PB296835
4. TITLE AND SUBTITLE ANALYSIS OF ORGANIC AIR POLLUTANTS BY GAS CHROMATOGRAPHY AND MASS SPECTROSCOPY Final Report		5. REPORT DATE March 1979 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Edo D. Pellizzari		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Research Triangle Institute P. O. Box 12194 Research Triangle Park, N.C. 27709		10. PROGRAM ELEMENT NO. 1AD712 BB-08 (FY-77) 11. CONTRACT/GRANT NO. 68-02-2262
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Sciences Research Laboratory-RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, North Carolina 27711		13. TYPE OF REPORT AND PERIOD COVERED Final 10/75-9/78 14. SPONSORING AGENCY CODE EPA/600/09
15. SUPPLEMENTARY NOTES		

16. ABSTRACT

Analytical methods and instrumentation for collecting and analyzing hazardous vapor-phase organics occurring in ambient air were developed and evaluated. The areas of investigation included (a) the evaluation of Tenax GC sorbent for variations in the breakthrough volumes for different lots; (b) studies on in situ reactions which might occur during the collection of organic vapors from ambient air; (c) evaluation of a permeation system for delivering precise quantities of organic vapors for calibrating instruments; (d) development of software programs for quantification of volatile organics using high resolution gas chromatography/mass spectrometry/computer (hrgc/ms/comp); (e) determination of relative molar response factors (RMR) for quantitative hrgc/ms/comp analysis; and (f) the identification and quantification of organic pollutants in ambient air from several geographical areas within the Continental U.S.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
*Air pollution *Organic compounds *Gas chromatography *Mass spectroscopy *Computers		13B 07C 07D 14B 09B

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 243
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE A11 - A01

EPA Form 2220-1 (9-73)

☆U.S. GOVERNMENT PRINTING OFFICE: 1979 -640-013/ 4216 REGION NO. 4

EPA-600/2-79-057
March 1979

ANALYSIS OF ORGANIC AIR POLLUTANTS BY GAS CHROMATOGRAPHY AND MASS SPECTROSCOPY

Final Report

by

Edo D. Pellizzari
Research Triangle Institute
Post Office Box 12194
Research Triangle Park, North Carolina 27709

Contract No. 68-02-2262

Project Officer

Kenneth Krost
Atmospheric Chemistry and Physics Division
Environmental Sciences Research Laboratory
Research Triangle Park, North Carolina 27711

ENVIRONMENTAL SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NORTH CAROLINA 27711

1a

DISCLAIMER

This report has been reviewed by the Environmental Sciences Research Laboratory, U. S. Environmental Protection Agency, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the U. S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

ABSTRACT

Development, perfection and evaluation of analytical methods and instrumentation for collecting and analyzing hazardous vapor-phase organics occurring in ambient air was conducted. The areas of investigation included (a) the evaluation of Tenax GC sorbent for variations in the breakthrough volumes for different lots; (b) studies on in situ reactions which might occur during the collection of organic vapors from ambient air; (c) evaluation of a permeation system for delivering precise quantities of organic vapors for calibrating instruments; (d) development of software programs for quantification of volatile organics using high resolution gas chromatography/mass spectrometry/computer (hrgc/ms/comp); (e) determination of relative molar response factors (RMR) for quantitative hrgc/ms/comp analysis; and (f) the identification and quantification of organic pollutants in ambient air from several geographical areas within the Continental U.S.

This report was submitted in fulfillment of contract No. 68-02-2262 by the Research Triangle Institute under the sponsorship of the U. S. Environmental Protection Agency. This report covers the period from November 10, 1975 to August 9, 1978 and work was completed as of August 9, 1978.

CONTENTS

Abstract iii
Figures vi
Tables viii
Acknowledgements xiv

1. Introduction 1
2. Conclusions 4
3. Recommendations 6
4. Program Objectives 8
5. Studies on Potential In Situ Reactions Occurring on Tenax GC Sorbent 9
6. Development of Methodology for Quantitative Analysis of Ambient Air Pollutants 25
7. Identification and Quantification of Organic Pollutants in Ambient Air from Several Geographical Area 67

References 116

Appendices

A. Method for Sampling and Analysis of Volatile Organic Compounds in Ambient Air by GC/MS/COMP 119
B. Volatile Organics Identified in Ambient Air 146
    Part I - Iberville Parish and Baton Rouge, LA 147
    Part II - Linden and Deepwater, NJ 177
    Part III - Camden, NJ-Philadelphia, PA 214

FIGURES

Number		Page
1	Research components encompassing analysis of organic vapors in ambient air by high resolution gas chromatography/mass spectrometry/computer (HRGC/MS/COMP)	2
2	Schematic of instrumentation and devices for examining *in situ* formation of halogenated hydrocarbons on solid sorbent surfaces	11
3	Linear regressions for benzene and phenylacetylene	35
4	Linear regressions for chlorobenzene and dichlorobenzene	36
5	Linear regressions for methylene chloride and chloroform	37
6	Linear regressions for toluene and ethyl acetate	38
7	Linear regressions for tetrachloroethylene	39
8	Area ratio calculation	42
9	Map depicting locations of ambient air sampling network in Iberville Parish, LA	77
10	Map depicting sampling locations near industrial complex in Iberville Parish, LA	78
11	Sampling site and locations for Baton Rouge, LA area	83
12	Sampling site and locations in Baton Rouge, LA	84
13	General location of American Cyanamid Corp. with respect to Tremley's Point and Staten Island	88
14	Sampling locations on American Cycnamid Corp. plant site	89
15	General location of E. I. DuPont de Nemours	90
16	Sampling locations on E. I. DuPont de Nemours plant site	91
17	Map of Chester, Camden, Philadelphia areas along the Delaware River	93
18	Mass spectrum of unknown (peak No. 46, Table B33) compound in ambient air from Linden, NJ	109

FIGURES

Number Page

A1 Vapor collection and analytical systems for analysis of organic vapors in ambient air. 121

A2 Sampling head for housing cartridge sampling train. 129

A3 Profile of ambient air pollutants for Wood River, IL using high resolution gas chromatography/mass spectrometry/computer 136

A4 Background profile for Tenax GC cartridge blank 137

A5 Schematic diagram of gc-ms computer system. 139

A6 Mass fragmentograms of characteristic ions representing carbon tetrachloride (m/e 117), tetrachloroethylene (m/e 166) and _m_-dichlorobenzene (m/e 146) in ambient air 142

A7 Mass fragmentograms of characteristic ions representing methylene chloride (m/e 49) and chloroform (m/e 83) in ambient air. 143

TABLES

Number | | Page
1 Operating Parameters for GLC-MS-COMP System. 13
2 Effects of Reactant Gases and Molecular Chlorine on *in situ* Formation of Halogenated Ethanes on Tenax GC . . 15
3 Effect of NO, NO_2 and O_3 on Chlorination of Ethylene . . . 16
4 Effects of Standard Pollutants, Molecular Chlorine, and Olefins on *In Situ* Formation of Halogenated Compounds on Tenax GC 17
5 Effect of NO, NO_2 and O_3 on Chlorination of Olefins. . . . 19
6 Effects of Reactant Gases and Molecular Bromine on *In Situ* Formation of Halogenated Ethanes on Tenax GC. 21
7 Effects of Reactant Gases and Molecular Bromine on *In Situ* Formation of Halogenated Ethanes on Tenax GC. 22
8 Effects of Standard Pollutants, Molecular Bromine, and Olefins on *In Situ* Formation of Halogenated Compounds on Tenax GC 23
9 Comparison of Breakthrough Volumes for Virgin, Virgin-Solvent Extracted and Recycled Tenax GC 27
10 Comparison of Permeation Rates at 20°C and 30°C for a Number of Selected Organics 29
11 Chemicals Selected for RMR Determinations. 44
12 Operating Parameters for GLC-MS-COMP System. 48
13 Statistical Data for Relative Molar Response Factor of Chloroform Based on M/Z 83 and M/Z 186 for Perfluorobenzene 50
14 Relative Molar Response for Normal Alkanes Using Selected Mass Ions 51
15 Relative Molar Response Factors for Statistical Deviations for Several Hydrocarbons and Aromatics Using Perfluorobenzene Standard. 52

TABLES

Number | | Page
16 Relative Molar Response Factors and Statistical Deviations for Chlorinated Hydrocarbons Using Perfluorobenzene Standard. 54
17 Relative Molar Response Factors and Statistical Deviations for Chlorinated Aromatics Using Perfluorobenzene Standard. 58
18 Relative Molar Response Factors and Statistical Deviations for Several Oxygenated Compounds using Perfluorobenzene Standard. 59
19 Relative Molar Response Factors and Statistical Deviations for Several Hydrocarbons and Aromatics Using Perfluorotoluene Standard. 60
20 Relative Molar Response Factors and Statistical Deviations for Methylene Chloride and Chloroform Using Perfluorotoluene Standard. 62
21 Relative Molar Response Factors and Statistical Deviations for Chlorinated Aromatics Using Perfluorotoluene Standard. 65
22 Relative Molar Response Factors and Statistical Deviations for Oxygenated Compounds Using Perfluorotoluene Standard. 66
23 Potential Emissions from Chemical Industry in Baton Rouge, LA. 68
24 Potential Organic Compounds Associated with E. I. DuPont de Nemours Facility (Chambers Works), Deepwater, NJ . 71
25 Representative Chemical Industry Along the Delaware River of the Camden, NJ and Philadelphia, PA Areas. . 72
26 Priority Organic Vapors Selected for Detection and/or Quantification in Ambient Air from Camden-Philadelphia Area 74
27 Ambient Air Sampling Protocol for Plaquemine, LA Area. . . 75
28 Ambient Air Sampling Protocol for Baton Rouge, LA Area . . 80
29 Key to Major Industrial Plants 85

TABLES

Number Page

30 Ambient Air Sampling Protocol for Linden and Deepwater, NJ. 86

31 Ambient Air Sampling Protocol for Camden/Philadelphia Area . 92

32 Summary of Volatile Halogenated Organics in Ambient Air from Iberville Parish in Louisiana. 95

33 Summary of Organic Vapors Identified in Ambient Air in Baton Rouge, LA and Vicinity. 97

34 Concentrations of Ambient Air Pollutants in Iberville Parish, LA. 100

35 Concentrations of Ambient Air Pollutants in Iberville Parish, LA. 101

36 Volatile Organic Vapors Estimated in Ambient Air of Baton Rouge, LA and Vicinity. 102

37 Minimum Total Halogenated Hydrocarbon Vapor in Ambient Air of Baton Rouge, LA. 103

38 Volatile Organics Identified in Ambient Air at American Cyanamid Co, Linden, NJ 105

39 Volatile Organics Identified in Ambient Air at E. I. DuPont de Nemours, Deepwater, NJ. 107

40 Ambient Air Levels of Several Volatile Organic Vapors Surrounding American Cyanamid Corp., Linden, NJ. 111

41 Ambient Air Levels of Several Volatile Organic Vapors Surrounding E. I. DuPont de Nemours, Deepwater, NJ 112

42 Estimation of Levels of Halogenated Hydrocarbons in the General Area of Camden, NJ/Philadelphia, PA 114

A1 Overall Theoretical Sensitivity of High Resolution Gas Chromatography/Mass Spectrometry/Computer Analysis for Atmospheric Pollutants. 122

A2 Tenax GC Breakthrough Volumes for Several Atmospheric Pollutants 130

A3 Operating Parameters for GLC-MS-COMP System. 135

TABLES

Number | | Page
B1 Volatile Organics in Ambient Air from Iberville Parish in Louisiana. 148

B2 Volatile Organics in Ambient Air from Iberville Parish in Louisiana. 149

B3 Volatile Organics in Ambient Air from Iberville Parish, Louisiana. 151

B4 Volatile Organics in Ambient Air from Iberville Parish, Louisiana. 153

B5 Volatile Organics in Ambient Air from Iberville Parish, Louisiana. 155

B6 Volatile Organics in Ambient Air from Iberville Parish, Louisiana. 157

B7 Volatile Organics in Ambient Air from Iberville Parish, Louisiana. 159

B8 Volatile Organics in Ambient Air from Iberville Parish, Louisiana. 161

B9 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #17. 162

B10 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #21. 163

B11 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #23. 165

B12 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #26. 167

B13 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #27. 169

B14 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #28. 171

B15 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #30. 173

B16 Volatile Organic Vapors in Ambient Air of Baton Rouge, LA at Location #26. 175

TABLES

Number / Page

B17 Volatile Organics in Ambient Air at American Cyanamid Corp. (P1/L1). 178
B18 Volatile Organics in Ambient Air at American Cyanamid Corp. (P1/L2). 181
B19 Volatile Organics in Ambient Air at American Cyanamid Corp. (P2/L1). 183
B20 Volatile Organics in Ambient Air at American Cyanamid Corp. (P2/L1). 185
B21 Volatile Organics in Ambient Air at American Cyanamid Corp. (P2/L3). 187
B22 Volatile Organics in Ambient Air at American Cyanamid Corp. (P3/L4). 189
B23 Volatile Organics in Ambient Air at E. I. DuPont (P4/L4). . 191
B24 Volatile Organics in Ambient Air at E. I. DuPont (P5/L1). . 193
B25 Volatile Organics in Ambient Air at E. I. DuPont (P5/L4). . 195
B26 Volatile Organics in Ambient Air at E. I. DuPont (P6/L1). . 197
B27 Volatile Organics in Ambient Air at E. I. DuPont (P6/L2). . 199
B28 Volatile Organics in Ambient Air at E. I. DuPont (P6/L8). . 201
B29 Volatile Organics in Ambient Air at American Cyanamid Corp. (P1/L1). 203
B30 Volatile Organics in Ambient Air at American Cyanamid Corp. (P1/L2). 205
B31 Volatile Organics in Ambient Air at American Cyanamid Corp. (P1/L4). 207
B32 Volatile Organics in Ambient Air at American Cyanamid Corp. (P1/L2). 209
B33 Volatile Organics in Ambient Air at American Cyanamid Corp. (P2/L3). 211
B34 Volatile Organics in Ambient Air at American Cyanamid Corp. (P3/L3). 212
B35 Volatile Organics Identified in Air in Bristol, PA (P1/LLA) 215

TABLES

Number — Page

B36 Volatile Organics Identified in Air in Bristol, PA (P1/L1B) 216

B37 Volatile Organics Identified in Ambient Air from North Philadelphia, PA (P3/L3A) 218

B38 Volatile Organics Identified in Ambient Air in Philadelpha, PA (P3/L3B) 220

B39 Volatile Organic Vapors Identified in Ambient Air from Philadelphia, PA (P4/L4B) 222

B40 Volatile Organics Identified in Ambient Air from Marcus Hook, PA (P5/L5A) 224

B41 Volatile Organics Identified in Ambient Air from Logan Township, NJ (P8/L8A) 227

ACKNOWLEDGEMENTS

The valuable assistance of Messrs. J. Bunch and R. Williams who performed laboratory and field experiments is gratefully appreciated. Ms. N. Castillo, D. Smith and Dr. J. T. Bursey provided expert interpretation of mass spectra and sample analyses, a sincere thanks for their support.

The author wishes to thank the personnel at EPA Regions II and VI, Texas Air Board, Louisiana Air Board, and the Department of Environment in New Jersey for their assistance throughout the program.

The constant encouragement of Mr. K. Krost and Dr. E. Sawicki are deeply appreciated.

SECTION 1
INTRODUCTION

During the past several years, research has been conducted on the development of a method for the collection and analysis of vapor-phase organics including carcinogenic and mutagenic substances (1-27). The developed techniques were to achieve a sensitivity of ng/m^3. While developing these techniques, it became apparaent that a number of facets required attention for successful completion of this concept. Figure 1 depicts these research components which encompass the analysis of organic vapors in ambient air using high resolution gas chromatography/mass spectrometry/computer (hrgc/ms/comp).

There have been two major areas of effort. One area involves the design and fabrication of devices while the second involves experimental evaluation. With regard to a collection method, design criteria and the preparation of appropriate sorbent media must be undertaken. These aspects have been previously discussed and reported (1-11). In addition, upon collection of organic vapors, a provision for their transfer to the instrumental method must be made. The design criteria, fabrication of an inlet manifold and associated capillary technology for use with mass spectrometry have also been briefly described (1-5,27). Finally, computer software must be developed with features which allow for rapid data interpretation.

Concommitant with the design and fabrication of devices, experimental evaluation has been conducted to varying degrees at each step of this method (Fig. 1). Collection efficiences, breakthrough volumes and research on displacement chromatography have been previously discussed (1-5). More recent work has centered on the examination of in situ reactions potentially associated with the collection device, as well as, the effects of storage on sample integrity. As an integral part of the instrumental method of analysis, the accuracy and reproducibility of sample recovery, and separation and resolution of components in the ambient air sample has been briefly

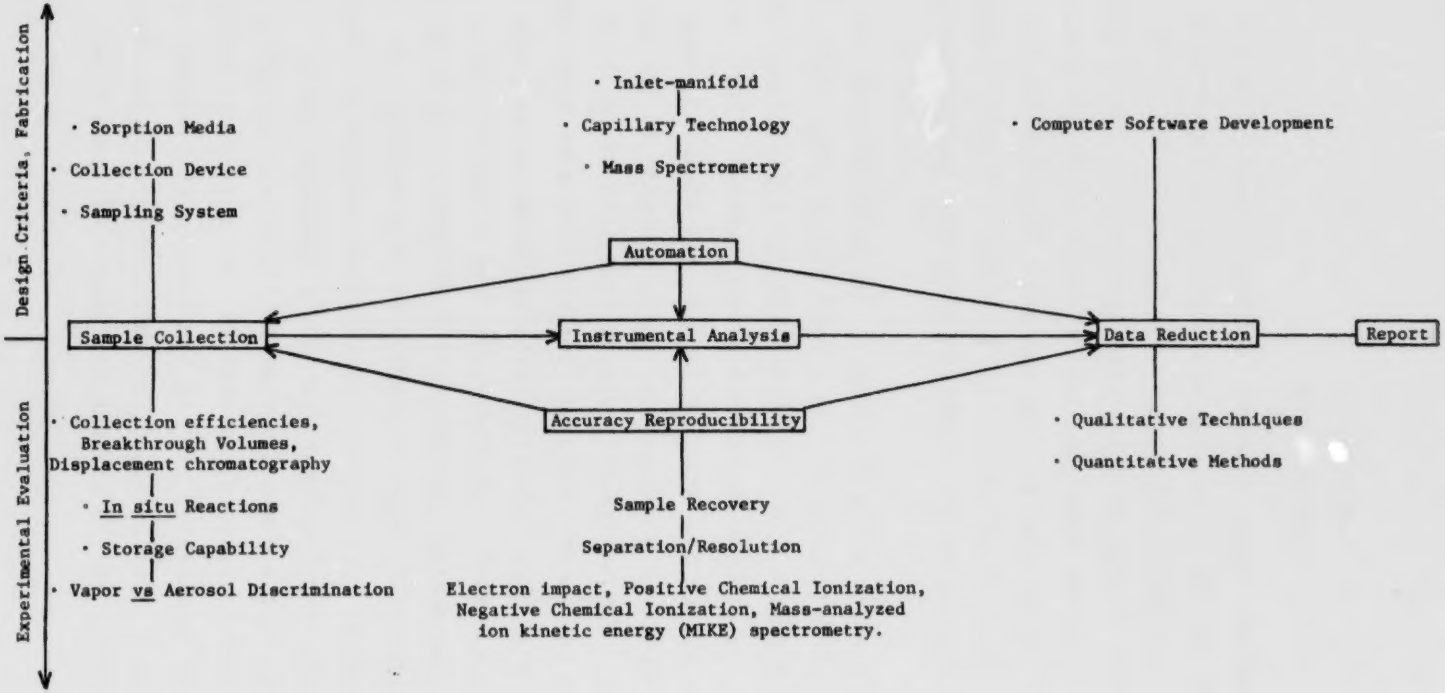

Design Criteria, Fabrication
Experimental Evaluation
· Sorption Media
· Collection Device
· Sampling System
Sample Collection
· Collection efficiencies, Breakthrough Volumes, Displacement chromatography
· In situ Reactions
· Storage Capability
· Vapor vs Aerosol Discrimination
· Inlet-manifold
· Capillary Technology
· Mass Spectrometry
Automation
Instrumental Analysis
Accuracy Reproducibility
Sample Recovery
Separation/Resolution
Electron impact, Positive Chemical Ionization, Negative Chemical Ionization, Mass-analyzed ion kinetic energy (MIKE) spectrometry.
· Computer Software Development
Data Reduction
· Qualitative Techniques
· Quantitative Methods
Report

Figure 1. Research components encompassing analysis of organic vapors in ambient air by high resolution gas chromatography/mass spectrometry/computer (HRGC/MS/COMP).

investigated (1-5). The assorted mass spectrometric techniques available for ambient air characterization includes electron impact, positive chemical ionization, negative chemical ionization, mass analyzed ion kinetic energy spectrometry as well as others. Virtually no research has been conducted with the latter three.

Finally, qualitative and quantitative techniques are needed for data reduction which expedites the overall sample analysis.

Many of the components in the two general areas outlined in Figure 1 have been examined over the past several years, however considerable effort is still required, in particular, their evaluation and validation.

To-date a considerable amount of qualitative and quantitative data has been accumulated utilizing the developed methods. Ambient air sampling has been conducted involving many types of industrial atmospheres located throughout the Continental U.S. (1-27).

In this report, we continue to provide information on experimental evaluation and validation of the previously developed methods as well as the acquisition of information on the composition of atmospheres asssociated with industrial activity.

SECTION 2
CONCLUSIONS

Studies were conducted on in situ reactions potentially occurring as a result of the presence of criteria pollutants (ozone, NO, NO_2, NO_x), molecular halogens and olefins occurring simultaneously in the atmospheres sampled. Under laboratory simulated conditions, no in situ reactions were observed when sampling atmospheres using a Tenax GC cartridge containing molecular chlorine or molecular bromine in the presence of criteria pollutants and ethylene, propylene and 1-butene. However, traces of 2,3-dichlorobutanes were detected from 2-butene. Also, very small quantities of 1,2-dichlorocyclohexane was detected as a reaction between chlorine and cyclohexene. The formation of these two halogenated hydrocarbons occurred under high levels of molecular chlorine and olefins. The incorporation of sodium thiosulfate into the glass fiber filter prior to a Tenax GC sampling cartridge for removing particulates inhibited the formation of chlorinated or brominated substances.

Development of computer software programs to assist in quantitation of the vapor-phase organics collected from ambient air substantially increased the efficiency of the overall technique. Two computer programs were developed, one provided the capability to sum ions representing classes of compounds over the mass spectra obtained in a gas chromatogram for a sample while the other provided the capability of determining the response (peak height or area) for a selected ion with subsequent ratioing of the intensity of the selected ion with respect to an internal standard to yield response factors as well as the quantity of the individual unknown component.

A series of relative molar response factors was determined for a number of hydrocarbons, aromatics, halogenated hydrocarbons and oxygenated compounds. The combined use of a permeation system for synthesizing air/vapor mixtures high resolution gas chromatography and mass spectrometry yielded RMR data for individual selected ions of each specific compound with a reproducibility of at least ±10% for replicate analysis. A statistical evaluation was conducted to compare the relative molar response factors within replicate determinations as well as to determine the variation of the RMR between compounds for the same selected ions. It was concluded that in some cases, ions common to several compounds within a homologeous series provided similar RMR values and thus an "average" RMR value could be used to extrapolate concentrations of compounds for which authentic material did not exist.

The collection and analysis techniques employing the Tenax GC cartridge and high resolution gas chromatography/mass spectrometry/computer was applied to the analysis of vapor-phase organics in ambient air for three major geographical areas (7 sites) in order to validate the technique by characterizing atmospheres where the composition of the industrial atmospheres was partially known. A group of halogenated hydrocarbons were identified in the atmospheres collected from the Houston, TX vicinity, Baton Rouge, LA area and New Jersey. Many of the compounds appeared to be site-specific. For example, some site-specific pollutants were chloroacetylene, vinyl chloride, chloroethane, vinylidene chloride, dichlorobutene isomers, 1,1,2-trichloroethane, bis(2-chloroisopropyl)ether, dichlorobutadiene isomers, 1,3-hexachlorodibutadiene, 1,3-dichloropropane, trichloropropene isomers, 1,1,2,2-tetrachloroethane, tetrachloropropane, hexachloroethane, perchlorobutadiene and chlorotoluene isomers which were identified in the Plaquemine, LA area. Other site-specific compounds were also detected in Geismar and Baton Rouge, LA Deer Park and Pasadena, TX and Deepwater and Linden, NJ.

SECTION 3
RECOMMENDATIONS

During the course of this research program, a number of areas have come to light which need further attention. Eleven major phases of research should be expanded and pursued. (1) New polymeric sorbent substances should be developed for the collection of the very polar hazardous substances which are not retained by Tenax GC. This may involve the synthesis of analogs which are modified polymer bases of Tenax in order to incorporate the desired retention volume properties for organics without increasing the overall background contribution and retention of inorganic gases and water. (2) Potential displacement chromatography should be examined for the sorbents Tenax GC and a new polymeric substance when it is developed under field sampling conditions. This information is needed in order to ascertain whether the breakthrough volumes that have been determined under ideal (laboratory) conditions are relevant to field sampling where high pollution may cause competition between pollutants for adsorption sites. (3) An evaluation of the collection media for in situ reactions with particular emphasis devoted to examination of potential artifacts under field sampling conditions. This activity should delineate problems associated with sampling of atmospheres containing molecular chlorine, bromine or iodine in combination with olefins, NO_x, SO_2 and ozone. Other potential in situ reactions on the sorbent bed should also be examined such as the ozonization of olefins under field sampling conditions. (4) An evaluation study should be made for drying the sorbent collection device albeit Tenax GC or a new synthesized polymer with a dehydrating agent such as calcium sulfate (or equivalent). Storage studies should be conducted to determine the accuracy and reproducibility of such a technique. (5) Further research is needed in regard to flow controls and the maintenance of a constant temperature on the sampling device to improve quantitative collection of atmopsheric vapors. Because the collection device is potentially subjected to variations in temperature and thus breakthrough volumes the use of a constant temperature bath for housing of the collection device should be investigated. This may include studies on the effects of condensation on collection efficiency and the storage of organic vapors on the sorbent medium. (6) Research should be initiated on evaluating the accuracy of the sampling device under field sampling conditions. This may require the use of radioisotopes incorporated in permeation tubes which are used to spike the endogenous organic pollutants followed by the subsequent determination of the accuracy of collection by measuring the radiotracer substance. (7) The reproducibility of storing the field collected organic vapors should be evaluated. This should include the reproducibility of storage for the individual components in the sample and the total organic vapor profile which was collected. (8) Substantial effort should be devoted to developing capillary technology for the analysis of hazardous (mutagenic, carcinogenic, toxic) substances collected from the ambient air. This should include the investigation of suitable stationary phases coated in glass capillary columns (SCOT and WCOT) as single pure phases as well as multiple phase combinations. (9) Research should begin on examining alternate methods to electron impact mass spectrometric techniques such as negation ion chemical ionization for halogenated hydrocarbons, selective chemical ionization for specific chemical classes, and mass analyzed ion kinetic energy (MIKE) spectrometry. (10) Evaluation and development of new qualitative and quantitative software techniques should be undertaken to handle large quantities of mass spectrometric data. This development and perfection should provide a single software package allowing for the characterization and quantitation of mass spectral information contained in a single sample run. Particular emphasis should be devoted to a capability which allows for bulk data processing at low cost. (11) Efforts should begin on developing concepts for overall automation of the developed collection and analysis methods for vapor-phase organic substances occurring in ambient air.

SECTION 4

PROGRAM OBJECTIVES

The general objective of this program was to fabricate the necessary instrumentation to collect and evaluate urban air samples using the services of a gas chromatograph in combination with a mass spectrometer. Preliminary emphasis was to be placed on developing a collection system of such sufficiency as to meet the sensitivity limitations of the analyzer combination. A major emphasis of this program was the quantitated determination of urban air organic pollutants. The specific aims of this program were: (a) to formulate a sample collection system which would permit in the minimum the analysis of pollutants in the vapor-phase present at low ng/m^3 concentrations. This included delineation of those parameters which are important in striving for a quantitative method of analysis; (b) demonstration of any limitations with regard to chromatographic resolution of urban air pollutants; (c) demonstration of the quantitative sensitivity of the overall collection and analysis systems for several classes of potential pollutant candidates, and (d) the analysis of vapor-phase ambient air pollutants by the use of gas chromatography in tandem with mass spectrometry with special emphasis on demonstrating the overall analysis method as a quantitative technique for atmospheric organic vapors which can be used concurrently with qualitative characterization.

SECTION 5

STUDIES ON POTENTIAL IN SITU REACTIONS OCCURRING ON TENAX GC SORBENT

An approach to the detection, identification and quantification of halogenated hydrocarbons in the ambient air has been previously described and has been further studied in this program (1-27). Ambient air was sampled using a Tenax GC cartridge technique and sample analysis employed high resolution (glass capillary) gas chromatography/mass spectrometry/computer (hrgc/ms/comp) methods. Many halogenated hydrocarbons have been identified and quantified in ambient air from several geographical regions throughout the Continental U.S.

In view of the potency and the broad spectrum of carcinogenic activity for the identified halogenated hydrocarbons in experimental animals, the detection of these compounds in the atmosphere has generated considerable interest in their origin. Many of the studies reported in Section 7 were initiated to determine their emission from stationary and fugitive sources as well as their potential formation through photochemical reaction from precursors.

In order to determine whether halogenated hydrocarbons may be present in the atmosphere from industrial sources or as an atmospheric chemical reaction, it was first necessary to know the extent to which it may form at trace levels as an "artifact" of the technique employed or the sample collection process. Furthermore, the experimental methods should differentiate between homogeneous and heterogeneous reaction mechanisms.

Our primary concern has been with the use of the Tenax GC sampling cartridge which has been extensively employed for collecting organic vapor from ambient air for characterization and quantification purposes. Since the Tenax GC cartridge may concentrate reactive compounds including ozone, NO_x and for example molecular chlorine or bromine, the possibility for *in situ* formation of artifact compounds may occur. This may occur eventhough inorganic gases do not appreciably accumulate on the sorbent (8). It was the purpose of this study to further supplement the previously reported observations, i.e., the in situ formation of N-nitrosamines, as to whether other additional in situ reactions could occur on the Tenax GC sampling cartridge (11,14).

Since urban air often contains substantial concentrations of ozone, we conducted a series of laboratory experiments to determine whether air containing both NO_x and ozone might be more effective in converting olefins plus molecular halogens than air containing only NO_x. Experiments were designed to delineate the transformation of olefins whether adsorbed on the Tenax GC or occurring in low concentrations in air via homogenous atmospheric reactions or heterogeneous reactions which might take place on the walls of the sample inlet tube. In addition to the halogenation of olefins, we were interested in the possibility of reactions between ozone and olefins producing polar products which also might be considered as artifacts of the collection process.

EXPERIMENTAL

The apparatus used to determine whether air containing ozone, NO (Matheson, Coleman, Bell), NO_2 (Matheson, Coleman, Bell), olefins, molecular halogens and water might convert olefins to halogenated compounds on Tenax GC (35/60, Applied Science, State College, PA) is depicted in Figure 2. Nitric oxide was measured into the stream with a rotameter and a metering valve from a supply tank which contained ppm of NO and nitrogen (Scott Environmental). Ozone was generated by an ultraviolet lamp equipped with a sliding cover for obtaining different concentrations. Concentrations of NO, NO_2 and ozone were monitored with a Bendix NO_x analyzer (Model 5513802) and a Bendix Ozone analyzer. Intakes for these instruments were at the same point as the intake for the Tenax GC glass cartridge sampler (1.5 cm i.d. x 6.0 cm bed length) through which air was drawn by a Nutech Model 221-A (Nutech Corp., Durham, NC) sampler. The sampling cartrige and the analyzer inlet tubes were centered in the air flow pattern from the reaction tube. Various levels of relative humidity in the air stream were produced by changing the temperature of the humdifier bath.

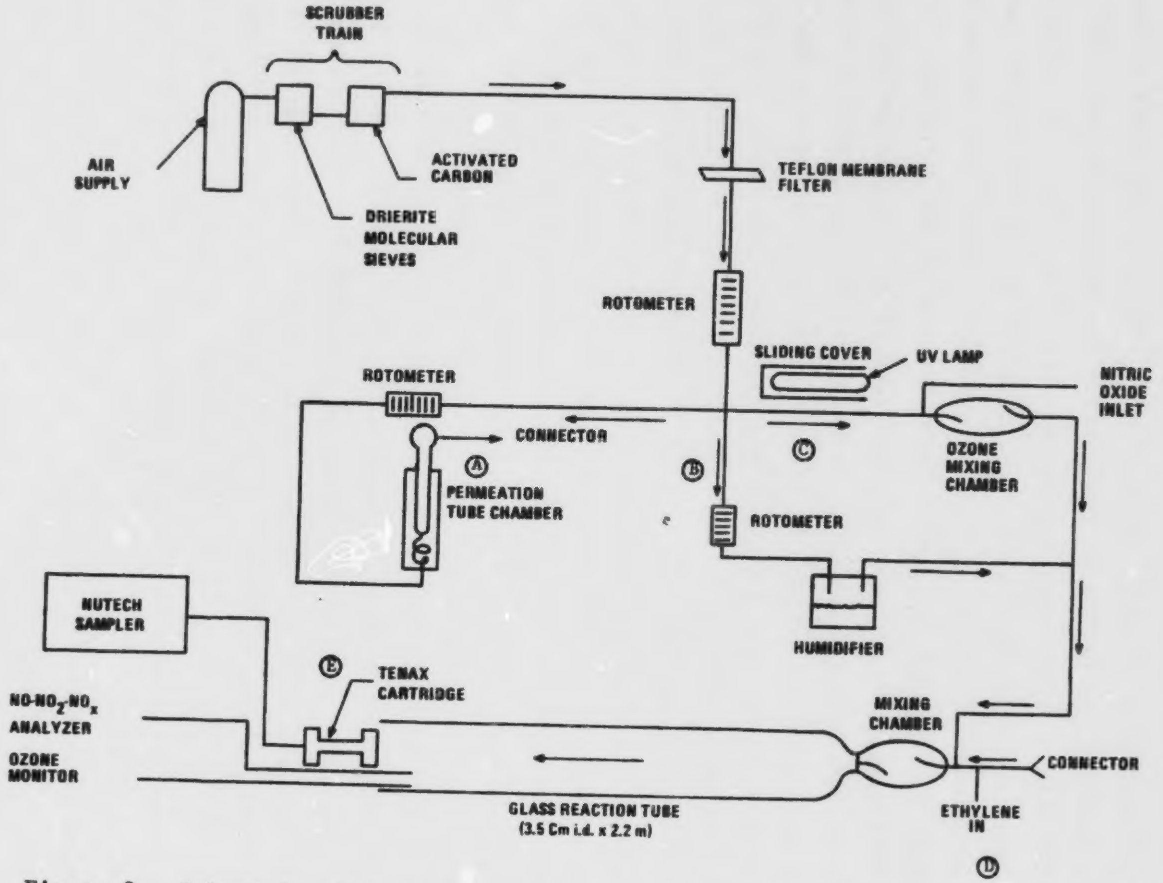

SCRUBBER TRAIN
AIR SUPPLY
ACTIVATED CARBON
DRIERITE MOLECULAR SIEVES
TEFLON MEMBRANE FILTER
ROTOMETER
SLIDING COVER
UV LAMP
NITRIC OXIDE INLET
ROTOMETER
CONNECTOR
A
PERMEATION TUBE CHAMBER
B
C
OZONE MIXING CHAMBER
ROTOMETER
HUMIDIFIER
NUTECH SAMPLER
E
TENAX CARTRIDGE
NO-NO$_2$-NO$_x$ ANALYZER
OZONE MONITOR
MIXING CHAMBER
CONNECTOR
GLASS REACTION TUBE (3.5 Cm i.d. x 2.2 m)
ETHYLENE IN
D

Figure 2. Schematic of instrumentation and devices for examining *in situ* formation of halogenated hydrocarbons on solid sorbent surfaces.

Permeation tubes (TFE) of molecular chlorine and bromine were prepared and gravimetrically calibrated with a MS-5A Mettler balance after their equilibration to a constant rate.

Prior to its use, Tenax GC was purified by Soxhlet extraction for 18 hrs with methanol and n-pentane, respectively. After drying under nitrogen atmosphere, Tenax GC was heated to 150°C for 2 hrs in a vacuum oven (12" of water), sized into a 35/60 range and packed into glass tubes. All sample cartridges were preconditioned by heating to 275°C for 20 min under a helium purge for 20-30 ml/min. After cooling in precleaned Kimax® culture tubes, the containers were sealed to prevent contamination of the cartridge.

Replicate samples and blanks were analyzed by gas chromatography equipped with flame ionization detection. Thermal desorption was used to transfer vapors from the cartridge sampler to the analytical system using a specially designed manifold (1-5). In a typical thermal desorption cycle, sampling cartridges were placed in the desorption chamber (275°C) and helium gas was passed through the cartridge (∿20 ml/min) to purge the vapors into the liquid nitrogen cooled nickel capillary trap. After desorption (4 min), the six-port valve was rotated and the temperature on the capillary loop was rapidly raised (>150°C/min). The carrier gas introduced the vapors onto the capillary glc column. The 100 m glass SCOT column containing OV-101 stationary phase and was programmed from 30°C to 240°C at 4°C/min.

A Varian MAT CH-7 glc/ms 620L computer system equipped with an inlet manifold was used for analyzing Tenax GC cartridges where structural confirmation was required. The software programs available with this system provides for reconstructed gas chromatograms and mass fragmentograms for correlation between mass spectrum number and retention time. Operating parameters for the hrgc/ms/comp system are given in Table 1. A single stage glass jet separator interfaced the SCOT capillaries to the mass spectrometer.

RESULTS AND DISCUSSION

A series of experiments were conducted which examined the potential in situ formation of chemical substances or their decomposition on the surface of the solid sorbent Tenax GC. The experimental conditions chosen were selected to allow the detection of potential in situ formation of organics

Table 1. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC	
100 m glass SCOT-OV-101	30-240°C, 4°C/min
carrier (He) flow	∿3 ml/min
transfer line to ms	240°C
MS	
scan range	*m/e* 20 → 300
scan range, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	6.0
ion source vacuum	∿4 x 10^{-6} torr

substances under typical atmospheric conditions encountered during field sampling.

Table 2 presents the series of experiments which were conducted utilizing different combinations of ozone, NO_x, NO, NO_2, chlorine and ethylene. The volume of air stream sampled was 16 ℓ in all cases. In all experiments (Expts. 1-15) with or without the presence of a glass fiber filter in front of the Tenax cartridge, no dichloroethane was detected. In Expt. 16-18, standard amounts of authentic dichloroethane were loaded onto cartridges to obtain a standard curve response for the flame ionization detector. The detection limit was ∿10 ng/cartridge.

Table 3 presents additional experiments on the effect of NO, NO_2 and ozone on chlorination of ethylene. In these experiments, higher concentrations of ozone were added to the extent that in some cases (Expt. 19 and 22) excess ozone was present. In other experiments, high concentrations of NO, and NO_2 were created to provide extreme atmospheric conditions to determine whether it was possible to produce chlorinated ethylene. As depicted in this table, no 1,2-dichloroethane or other products as the results of reactions between these reagent gases could be detected. The detection limit was ∿10 ng using a flame ionization detector.

Table 4 presents experiments employing various concentrations of standard pollutants and a mixture of olefins. Other olefins which might be more reactive were used to determine whether any halogenated hydrocarbons might be formed. The olefin mixture consisted of ethylene (10 ppm), propylene (9.92 ppm), 1-butene (12.8 ppm), *cis*-2-butene (7.82 ppm) and *trans*-2-butene (8.40 ppm). The flow rate was 250 ml/min into the mixing chamber prior to the reaction tube. Thus the various concentrations of olefins as indicated in Table 4 were produced. These olefin concentrations and the relative proportions remained the same for all experiments (Table 4). Molecular chlorine was introduced from a permeation tube (Metronix Assoc. Inc.) which had been calibrated to determine its permeation rate.

Again, no dichloroethane was detected in these experiments (Table 4). However, 2,3-dichlorobutanes (racemic and meso forms) were detected. Their formation also occurred in the absence of standard pollutants (Expt. 3). Indicated in this table are the relative amounts of each product based upon

Table 2. EFFECTS OF REACTANT GASES AND MOLECULAR CHLORINE ON IN SITU FORMATION OF HALOGENATED ETHANES ON TENAX GC

Experiment No.	Reactant Gas Concentrations (ppb)							Volume Sampled (ℓ)	$C_2H_4Cl_2$ detected (ng)	Remarks
	O (added)	O_3 (excess)	NO_x	NO	NO_2	Cl_2	C_2H_4			
1	0	0	C	0	0	86	590	16	ND	Blank control
2	0	0	0	0	0	0	0	16	ND	
3	0	0	0	0	0	86	0	16	ND	
4	0	0	0	0	0	86	590	16	ND	
5	160	160	0	0	0	86	590	16	ND	
6	250	120	130	0	130	86	590	16	ND	
7	880	880	0	0	0	86	590	16	ND	
8	1290	570	720	0	720	86	590	16	ND	
9	0	0	200	200	0	86	590	16	ND	
10	0	0	800	800	0	86	590	16	ND	
11	840	0	1720	880	840	86	590	16	ND	
12	740	740	0	0	0	86	590	16	ND	With GFF
13	1220	620	600	0	600	86	590	16	ND	With GFF
14	0	0	920	920	0	86	590	16	ND	With GFF
15	760	0	1520	760	60	86	590	16	ND	With GFF
16	-	-	-	-	-	-	-	-	840	S for response curve
17	-	-	-	-	-	-	-	-	420	
18	-	-	-	-	-	-	-	-	210	

Table 3. EFFECT OF NO, NO_2, and O_3 ON CHLORINATION OF ETHYLENE

Experiment No.[a]	O_3 Added (ppb)	O_3 Excess (ppb)	NO_x (ppb)	NO (ppb)	NO_2 (ppb)	Cl_2 (ppb)	C_2H_4 (ppm)	Vol. Sampled (ℓ)	1,2-dichloroethane (ng)
19	840	840	0	0	0	86	2.04	16	0
20	900	0	900	0	900	86	2.04	16	0
21	0	0	840	840	0	86	2.04	16	0
22	1020	520	500	0	500	86	2.04	16	0
23	600	0	1320	720	600	86	2.04	16	0

[a] Relative humidity = 50%, no GFF was used, sampling rate = 1 liter/min and all reactants and Cl_2 were introducted at beginning of flight tube (see Quarterly No. 5, Fig. 1).

Table 4. EFFECTS OF STANDARD POLLUTANTS, MOLECULAR CHLORINE, AND OLEFINS ON IN SITU FORMATION OF HALOGENATED COMPOUNDS ON TENAX GC

	Reactant Gas Concentration (ppb)															
Experiment No.	O_3 (added)	O_3 (excess)	NO_x	NO	NO_2	Cl_2	C_2H_4	C_3H_6	C_4H_8	C_4H_8 (cis)	C_4H_8 (trans)	Volume Sampled (ℓ)	2,3-DCB (rac.) detected Peat Ht. (cm)	2,3-DCB (Meso) detected Peak Ht. (cm)	$C_3H_6Cl_2$ (ng)	$C_2H_4Cl_2$
1	0	0	0	0	00	86	581	577	744	455	488	16	0	0	0	0
2	0	0	0	0	00	86	581	577	744	455	488	16	0	0	0	0
3	0	0	0	0	00	86	581	577	744	455	483	16	10.2	8.2	0	0
4	120	120	0	0	00	86	581	577	744	455	488	16	6.0	4.8	0	0
5	860	860	0	0	00	86	581	577	744	455	488	16	2.9	2.9	0	0
6	0	0	200	200	00	86	581	577	744	455	488	16	2.9	2.2	0	0
7	0	0	940	940	o	86	581	577	744	455	488	16	6.8	5.5	0	0
8	200	0	200	0	200	86	581	577	744	455	488	16	6.5	5.4	0	0
9	920	0	920	0	920	86	581	577	744	455	488	16	7.3	5.9	0	0

peak height response to the flame ionization detector. These results suggest that small quantities of chlorinated substances may be produced when molecular chlorine and 2-butenes (with or without standard pollutants) are presented to a Tenax GC sampling cartridge.

Table 5 presents experiments concerning the effect of NO, NO_2 and ozone on the chlorination of olefins (581 ppb ethylene, 577 ppb propylene, 744 ppb 1-butene, 455 ppb cis-2-butene and 488 trans-2-butene were the chamber concentrations). Ethylene, propylene and 1-butene did not yield detectable chlorinated hydrocarbons (detection limits ∿10 ng using flame ionization). On the otherhand, significant quantities of 2,3-dichlorobutane (racemic and meso) were detected. In the absence of ozone, NO_x, NO and NO_2 molecular chlorine and 2-butene did react whether it was introduced immediately in front of the Tenax GC cartridge or in the front of the flight tube to produce dichlorobutane mixtures (Expt. 17). On the otherhand, the addition of NO to the reaction between chlorine and 2-butene appeared to suppress the chlorination reaction (Expt. 12). In cases in which ozone was added or ozone plus NO, NO_2, low yields of chlorinated butanes were found.

Experiments 18-22, 24 and 28-31 were conducted in which the olefins were introduced at the beginning of the flight tube and sampling was conducted using a glass fiber filter impregnated with 10% sodium thiosulfate in front of the Tenax GC cartridge. In all of these experiments, regardless of the concentration of ozone, NO_x, and NO_2, no chlorinated products were detected. These experiments are contrasted with Expts. 23 and 27 which a glass fiber filter was used which had not been impregnanted with sodium thiosulfate.

The capacity of filters which have been impregnated with 10% sodium thiosulfate was tested using an ozone concentration of 200 ppb. A volume of 400 ℓ of air was pulled through the filter. The filter was then placed inline with the ozone monitor and no ozone was detected. The filter was not tested to its breakthrough limit since field sampling does not generally exceed a sampling volume of 200 ℓ and ozone levels seldom exceed 200 ppb.

The reaction products from the reactions between NO, NO_2 and ozone, chlorine and butene appear to increase by removing the glass wool plug which

Table 5. EFFECT OF NO, NO_2, and O_3 ON CHLORINATION OF OLEFINS

Experiment No.	Condition(s)[a]	O_3 Added (ppb)	O_3 Excess (ppb)	NO_x (ppb)	NO (ppb)	NO_2 (ppb)	Cl_2 (ppb)	2-butene (ppb)	2,3-dichlorobutane formed (rac.) (ng)	2,3-DCB(Meso) (ng)	Polar Material (pk. hgt., cm)
10	A	860	860	0	0	0	86	943	200	165	26
11	A	860	860	0	0	0	0	954	0	0	22
12	A	0	0	840	840	0	86	936	32	27	0
13	A	880	0	880	0	880	86	936	50	32	0
14	A	100	100	0	0	0	86	943	217	185	16
15	A	100	0	100	0	100	86	942	182	147	0
16	A	200	100	100	0	100	86	942	152	115	21
17	A	0	0	0	0	0	86	943	365	320	0
18	B	200	200	0	0	0	86	943	0	0	0
19	B	220	220	0	0	0	86	943	0	0	0
20	B	200	200	0	0	0	0	954	0	0	0
21	B	200	200	0	0	0	0	954	0	0	0
22	B	0	0	0	0	0	0	954	0	0	0
23	C	200	200	0	0	0	86	943	15	10	16
24	B	200	200	0	0	0	86	943	0	0	0
25	D	200	200	0	0	0	86	943	260	210	22
26	E	0	0	0	0	0	86	943	62	40	0
27	C	200	200	0	0	0	0	954	0	0	22
28	B	0	0	200	200	0	86	940	0	0	0
29	B	200	0	200	0	200	86	940	0	0	0
30	B	400	200	200	0	200	86	940	0	0	0
31	B	200	0	400	200	200	86	940	0	0	0

[a] A = olefins introduced immediately in front of cartridge (see Quarterly No. 5, Fig. 1).
B = olefins introduced at beginning of flight tube, GFF impregnated with 10% $Na_2S_2O_3$ was used.
C = olefins introduced at beginning of flight tube, GFF used.
D = olefins introduced at beginning of flight tube, glass wool used to anchor Tenax was removed.
E = olefins introduced at beginning of flight tube.

was used to anchor the Tenax or when the glass fiber filter on the intake to the Tenax cartridge was removed. The presence of the glass wool and glass fiber filter thus appeared to decrease the amount of artifact since seen which is in contrast to observations on the in situ reactions for the formation of N-nitrosamines (14). These observations indicate that the artifact reaction occur on the Tenax sorbent to a significant extent since yield as high as 300 ng were observed.

Furthermore, an additional artifact apparently occurred as indicated by the presence of polar compound during gas chromatography. In Table 5, the amount of polar material formed based upon peak height is given for the various experiments conducted. The polar material was identified subsequently by gc/ms to be propionic acid. Traces of acetone, acetic acid, acetaldehyde, propionaldehyde and methyl ethyl ketone were also detected. Formation of the major polar compound was also prevented using a sodium thiosulfate impregnated filter. New artifacts as the result of the impregnation of the glass fiber filter with sodium thiosulfate were not observed.

Potential in situ reaction experiments have also been conducted using ethylene and bromine. No artifacts have been observed. The detection limit for ethylene dibromide was approximately 50 ng when using flame ionization detection. Tables 6 and 7 present the effects of reagent gases and molecular bromine on in situ formation of halogenated ethanes on Tenax GC.

Table 8 gives the effects of standard pollutants, molecular bromine and olefins on in situ formation of halogenated compounds on Tenax GC. For the combination of reactive gases plus the olefin mixture as listed in the Expts. 1-16, no 2,3-dibromobutane was detected.

These results suggest that the formation of 2,3-dichlorobutane to be a rather unusual reaction since no other olefins appear to react with molecular chlorine and bromine in the presence or absence of criteria pollutants. The incorporation of sodium thiosulfate into the glass fiber filter may provide a new avenue for eliminating potential in situ formation reactions as a results of the presence of molecular halogens and/or ozone. It would be interesting to conduct further studies in light of these new observations as to whether the in situ formation of nitrosamines can be eliminated or

Table 6. EFFECTS OF REACTANT GASES AND MOLECULAR BROMINE ON IN SITU FORMATION OF HALOGENATED ETHANES ON TENAX GC

Experiment No.[a]	Reactant Gas Concentrations (ppb)							Volume Sampled (ℓ)	1,2-Dibromoethane ng
	O_3 (added)	O_3 (excess)	NO	NO_2	NO_x	Br_2	C_2H_4		
1	0	0	0	0	0	45	2,000	16	0
2	0	0	0	0	0	45	2,000	16	0
3	200	200	0	0	0	45	2,000	16	0
4	0	0	0	0	0	45	2,000	16	0
5	0	0	100	0	100	45	2,000	16	0
6	140	0	0	140	140	45	2,000	16	0
7	600	600	0	0	0	45	2,000	16	0

[a] Expt. Nos. 1-3 and 5 did not employ a glass fiber filter; Expts. 4, 6, 7 used $Na_2S_2O_3$ impregnated glass fiber filters.

Table 7. EFFECTS OF REACTANT GASES AND MOLECULAR BROMINE ON IN SITU FORMATION OF HALOGENATED ETHANES ON TENAX GC

Experiment No.[a]	Reactant Gas Concentrations (ppb)							Volume Sampled (ℓ)	1,2-Dibromoethane ng
	O_3 (added)	O_3 (excess)	NO	NO_2	NO_x	Br_2	C_2H_4		
1	0	0	0	0	0	45	2,000	16	0
2	0	0	0	0	0	45	2,000	16	0
3	200	200	0	0	0	45	2,000	16	0
4	0	0	0	0	0	45	2,000	16	0
5	0	0	100	0	100	45	2,000	16	0
6	140	0	0	140	140	45	2,000	16	0
7	600	600	0	0	0	45	2,000	16	0

[a] Expt. Nos. 1-3 and 5 did not employ a glass fiber filter; Expts. 4, 6, 7 used $Na_2S_2O_3$ impregnated glass fiber filters.

Table 8. EFFECTS OF STANDARD POLLUTANTS, MOLECULAR BROMINE, AND OLEFINS ON IN SITU FORMATION OF HALOGENATED COMPOUNDS ON TENAX GC

Experiment No.[a]	Reactant Gas Concentration (ppb)						Olefin Mix.[b]	Volume Sampled (ℓ)	2,3-Dibromobutane ng
	O_3 (added)	O_3 (excess)	NO	NO_2	NO_x	Br_2			
1	0	0	0	0	0	0	+	28	0
2	0	0	0	0	0	45	+	28	0
3	140	140	0	0	0	45	+	28	0
4	0	0	120	0	120	45	+	28	0
5	0	0	0	120	120	45	+	28	0
6	0	0	100	120	220	45	+	28	0
7	800	800	0	0	0	45	+	28	0
8	760	0	760	0	760	45	+	28	0
9	540	0	260	540	800	45	+	28	0
10	700	0	0	700	700	45	+	28	0
11	1200	600	0	600	600	45	+	28	0
12	700	700	0	0	0	45	+	28	0
13	600	400	0	200	200	45	+	28	0
14	600	0	150	600	750	45	+	28	0
15	0	0	600	0	600	45	+	28	0
16	0	0	0	0	0	45	+	28	0

[a] A glass fiber filter impregnated with $Na_2S_2O_3$ was used in each experiment.

[b] Olefin mixture = ethylene (580 ppb), propylene (580 ppb), 1-butene (740 ppb), cis 2-butene (455 ppb) and trans-2-butene (490 ppb).

suppressed by the incorporation of a sodium thiosulfate or an equivalent material impregnated into the filter prior to analysis.

SECTION 6

DEVELOPMENT OF METHODOLOGY FOR QUANTITATIVE ANALYSIS OF AMBIENT AIR POLLUTANTS

As discussed earlier there are many facets (Fig. 1) in the development of a technique for the analysis of organic vapors in ambient air by high resolution gas chromatography/mass spectrometry/ computer (hrgc/ms/comp). Among the experimental parameters which need evaluation in order to ascertain whether a method can become a quantitative tool are collection efficiency and breakthrough volumes for the sorbent medium under consideration, sample recovery and transfer to the analytical system, and development of methods for data reduction to obtain concentrations of individual components which originally occurred in the sample. This section addresses aspects of the method for quantitative analysis of ambient air pollutants by hrgc/ms/comp.

DETERMINATION AND COMPARISON OF BREAKTHROUGH VOLUMES FOR VIRGIN AND RECYCLED TENAX GC

Introduction

During the past few years, the density of commercially available virgin Tenax GC has decreased considerably. We addressed the possibility as to whether the previously determined breakthrough volumes were also decreasing with a decrease in density. In order to test this possibility, three batches of Tenax were examined. These were: virgin, virgin solvent-extracted and recycled sorbent.

Experimental

Virgin Tenax GC was purchased from Applied Science (State College, PA). Also Tenax GC purchased from the same source which had been recycled more than twenty times and was more than three years old was selected for evaluation.

Breakthrough volumes for five chemicals were determined using previously described techniques (5,8). The elution volume for vapors was determined on a chromatographic column at several decreasing temperatures and by the use of linear regression analysis. Extrapolation to ambient temperatures allowed the calculation of breakthrough volumes. The ambient temperature selected for comparison of breakthrough volumes between the different batches of Tenax was 21.1°C.

Virgin Tenax GC was also extracted in a Soxhlet apparatus for 18 hrs each with methanol and n-pentane, respectively. The recycled Tenax GC (> 3 years in age) was also solvent extracted prior to use in this study. All solvent was sized to 35/60 mesh before testing.

Results and Discussion

Comparison of breakthrough volumes for virgin, virgin-solvent extracted and recycled Tenax GC is given in Table 9. The breakthrough volumes were expressed in ℓ/g and in ℓ/cartridge volume. By comparing the three batches of Tenax using these units of expression, changes in the breakthrough volume from one batch to another whether it depended upon the density or surface area could be determined. For methylene chloride, a variation as large as 14% was observed between virgin and virgin solvent-extracted. A 30% difference was observed for the breakthrough volume for n-hexane between virgin and recycled Tenax. In general, the breakthrough volume of Tenax GC appeared to be lower for the material which had been recycled (and had the highest density) as compared to virgin or virgin solvent-extracted batches. The least variation was changes observed between virgin and virgin solvent-extracted sorbent. No changes were detected in the breakthrough volume values between the originally purchased Tenax and the same material which had been recycled for more than 3 years.

Recently purchased Tenax vs that which was several years old, exhibited 32% lower density.

These results indicate that the breakthrough volumes for organic vapors on Tenax GC may decrease or differ slightly between batches. This phenonmen complicates quantification using this sorbent and thus a dual cartridge system should be used, i.e. two cartridges in tandem

Table 9. COMPARISON OF BREAKTHROUGH VOLUMES FOR VIRGIN, VIRGIN-SOLVENT EXTRACTED AND RECYCLED TENAX GC[a]

Compound	B.P. °C	Virgin		Virgin/Extracted[b]		Recycled[c]	
		ℓ/g	ℓ/cart.	ℓ/g	ℓ/cart.	ℓ/g	ℓ/cart.
Methylene chloride	41	5.34	7.04	5.01	6.57	2.97	6.6
n-Hexane	68.7	41.83	55.14	37.41	49.13	7.58	17.0
n-Propylmercaptan	67.8	29.07	38.33	28.35	37.14	22.27	49.0
Benzene	80.1	65.55	85.09	63.63	83.35	24.64	54.0
Methyl ethyl ketone	80.2	36.32	47.87	35.29	46.23	17.89	39.0

[a] Breakthrough volumes are at 21.1°C.

[b] Virgin Tenax GC was extracted with methanol and n-pentane in a soxhlet for 18 hrs, respectively.

[c] Tenax sorbent that had been re-used for more than 20 times and was purchased at least three years ago was selected for testing.

should be employed during field sampling so that the amounts of organic vapors on the first and second cartridge can be determined and related to breakthrough volume under field sampling conditions. Using this approach, the variation in the breakthrough volumes between lots of Tenax as well as any variation in displacement of organic vapors occurring as a competitive adsorption-desorption process can be evaluated. A higher degree of accuracy and reproducibility in quantitative studies using this sorbent can be expected with this approach.

COMPARISON AND EFFECT OF TEMPERATURE (20°C and 30°C) ON PERMEATION RATES THROUGH PLASTIC MATERIALS

Introduction

In previous reports (4,5), a permeation system was described for the generation of air/vapor mixtures of known concentrations. The permeation system was designed to operate at 20°C, however adsorption of organic vapors to the glass surfaces and teflon transfer lines was experienced and thus a study was undertaken to ascertain whether the permeation system might function adequately at a higher temperature (e.g. 30°C).

Experimental

The design of the flow system was previously described (4,5). The pyrex permeation tube (25 mm i.d. x 44 cm in length) was enclosed in the jacket through which an ethanol/water mixture was circulated from a constant temperature bath (Haake Model FE Circulating Bath and Thermostated Heater). The thermostated heater was set to control the temperature at 30°C ± 0.1°C.

The permeation tubes were gravimetrically calibrated on a weekly basis. A Mettler MS-5A (microgram) balance was used.

Results and Discussion

Table 10 presents the permeation rates for a series of hydrocarbons, halogenated hydrocarbons, aromatics, nitrogen- and oxygen-containing compounds at 20°C and 30°C. In general, there is a 2-4 fold increase in the permeation rate between the two temperatures; however, this increase did not interfere with the utilization of the permeation tubes at their new permeation rates. Furthermore, it is desirable to have the permeation rates adjusted for each

Table 10. COMPARISON OF PERMEATION RATES AT 20°C and 30°C FOR A NUMBER OF SELECTED ORGANICS

Chemical Class	Compound	Tube Length/Material[a]	g/min	
			20°C	30°C
Halogenated Hydrocarbons	methylene chloride	11 cm FEP	3.1494×10^{-7}	6.9766×10^{-7}
	trichloroethylene	7.5 cm FEP		
	chloroform	10.2 cm TFE	1.245×10^{-6}	1.8707×10^{-6}
	m-dichlorobenzene	6 cm TFE	1.9346×10^{-7}	2.9794×10^{-7}
	m-dichlorobenzene	5.8 cm FEP	6.8197×10^{-9}	1.5697×10^{-8}
	1,1,1-trichloroethane	8 cm TFE	3.4207×10^{-8}	8.3768×10^{-8}
	tetrachloroethylene	5.2 cm TFE	1.8949×10^{-7}	4.3178×10^{-7}
	chlorobenzene	5.5 cm TFE	1.5523×10^{-7}	2.2901×10^{-9}
	carbon tetrachloride	8 cm PE w/ glass reservoir	6.0834×10^{-6}	1.2400×10^{-5}
	1,2-dichloroethane	8 cm TFE	2.0001×10^{-7}	4.3466×10^{-7}
	1,2-dichloropropane	7.7 cm TFE	1.4369×10^{-8}	1.9207×10^{-7}
	bis-2-chloroethyl ether	8.3 cm TFE	1.7441×10^{-8}	2.8220×10^{-8}
	2-chloro-1,3-butadiene (chloroprene)	9.5 cm TFE	6.7380×10^{-8}	1.7908×10^{-7}
	3-chloro-1-butene	9 cm TFE	2.8736×10^{-7}	3.2487×10^{-7}
	perfluorobenzene	2.5 cm FEP w/ glass reservoir		6.3748×10^{-6}

(continued)

Table 10 (cont'd)

Chemical Class	Compound	Tube Length/Material	g/min	
			20°C	30°C
	perfluorotoluene	4.5 cm FEP w/ glass reservoir		3.7115×10^{-6}
	dibromomethane	6.4 cm FEP	8.3052×10^{-8}	9.3067×10^{-8}
	dibromomethane	6.2 cm TFE	1.4219×10^{-6}	9.2725×10^{-7}
	methyl bromide	6 cm FEP	5.9383×10^{-7}	1.3174×10^{-6}
	1,2-dibromopropane	9.8 cm TFE	1.6811×10^{-7}	2.4410×10^{-7}
	bromodichloromethane	5.7 cm FEP	5.8948×10^{-9}	4.1538×10^{-8}
	bromodichloromethane	5.2 cm TFE	3.9341×10^{-7}	1.2473×10^{-7}
	1-bromo-2-chloroethane	9.8 cm TFE	1.7104×10^{-7}	3.3472×10^{-7}
Hydrocarbons	*n*-heptane	12.3 cm TFE	2.0605×10^{-7}	6.6725×10^{-7}
	1-pentyne	10 cm TFE	4.3353×10^{-7}	7.9355×10^{-7}
	cyclopentane	12.25 cm TFE	8.8957×10^{-9}	1.8092×10^{-7}
Aromatics	benzene	12.5 cm TFE	2.4087×10^{-7}	5.0473×10^{-7}
	toluene	7 cm TFE	1.0819×10^{-7}	2.0214×10^{-7}
	benzene-d_6	8 cm TFE	1.7034×10^{-7}	3.9505×10^{-7}
	benzene-d_6	8 cm FEP	2.8003×10^{-7}	1.8680×10^{-7}
	α-methylstyrene	13.9 cm TFE	2.4886×10^{-8}	9.4223×10^{-8}
	1,2,3-trimethylbenzene	13.7 cm TFE	5.1066×10^{-8}	2.3030×10^{-8}
	phenylacetylene	6 cm TFE	3.8153×10^{-8}	8.7830×10^{-8}

(continued)

Table 10 (cont'd)

Chemical Class	Compound	Tube Length/Material	g/min	
			20°C	30°C
Nitrogenous	dimethyl-d_6-amine	8 cm FEP	2.6297×10^{-7}	8.2204×10^{-7}
	dimethylamine	7 cm FEP	9.7171×10^{-8}	1.2606×10^{-7}
	dimethylamine	7 cm TFE	5.2915×10^{-7}	1.1500×10^{-6}
	dimethyl-d_6-amine	7.5 cm TFE	7.5030×10^{-7}	1.5886×10^{-6}
	N,N-dimethylformamide	8.75 cm TFE	3.9659×10^{-8}	4.5242×10^{-8}
	benzonitrile	9.75 cm TFE	2.6366×10^{-7}	3.2857×10^{-7}
Oxygenated	acetone	12.5 cm TFE	3.8730×10^{-7}	8.0447×10^{-7}
	methyl ethyl ketone	4.8 cm PE w/ glass reservoir	1.1901×10^{-6}	2.7582×10^{-6}
	methyl vinyl ketone	8.6 cm TFE	1.5982×10^{-7}	6.4973×10^{-8}
	ethyl acetate	2.8 cm PE w/ glass reservoir	1.3092×10^{-6}	3.2589×10^{-6}
	methyl acrylate	6.9 cm TFE	4.7977×10^{-7}	1.0020×10^{-6}
	furan	6.2 cm TFE	8.5109×10^{-7}	1.7729×10^{-6}
	_n_-butyl ether	6.2 cm TFE	8.1499×10^{-8}	9.6937×10^{-8}
	t-amylalcohol	6.9 cm PE	4.5901×10^{-8}	3.5927×10^{-7}
	heptanal	10.1 cm TFE	2.4886×10^{-8}	1.0980×10^{-8}

[a] TFE = tetrafluoroethylene polymer, PE = polyethylene, FEP = fluorinated ethylene (perfluoro).

organic compound to within 1 x 10^{-6} to 5 x 10^{-7} g/min. Permeation rates in this range are convenient for loading vapors onto Tenax GC cartridges.

Since it had been previously observed that substantial quantities of the less volatile organic vapors (e.g. chlorobenzene) were adsorbed to the surfaces of the permeation system, accurate delivery of vapors to the Tenax GC cartridges was not possible. By increasing the temperature of the permeation system to 30°C and then subsequently maintaining the transfer lines to the Tenax GC cartridges at $\geq$ 40°C, the adsorption of the less volatile vapors to the surface of the system were minimized.

EXAMINATION OF THE COMBINED PERFORMANCE OF THE PERMEATION SYSTEM, INLET-MANIFOLD, AND HIGH RESOLUTION GAS-LIQUID CHROMATOGRAPHY

Introduction

In a previous report (4), modifications to a flow system for delivering vapors from a permeation tube to Tenax cartridges for the purpose of accurately loading cartridges to calibrate instruments were described. In that study the performance of the flow system was evaluated in terms of stability of the signal from the flame ionization detector (FID) with respect to the criteria, of noise and drift. Noise was defined as variations in the signal level over a period of 15 sec or less and it consisted substantially of oscillations about the mean signal level. This noise was expressed as the percentage of the lowest observed signal level. Part of the noise originated in the FID electrometer but some of it also originated in the flow system. Drift consisted of variations in signal level over a period exceeding 15 sec. It also was expressed as a percentage of the lowest observed signal level. The noise and drift problems were believed to be due to the instability of the pressure and flow through the air/vapor permeation device. Modifications were made in the regulation of the flow and pressure in this system. Noise was minimal and drift was slight except for one observation which lasted for about 4 1/2 hrs. The behavior of the signal level when changing from one Tenax cartridge to another was observed at pressures up to 6 in of water. No significant flucuations and signal level occurred at 4 in of water and above. The influence of pressure on the time required for this signal level to stabilize after insertion of permeation tubes into the system was also observed and found to be insignificant. The signal level approached its final level within 20 min and sometimes required a short additional period to completely stabilize.

It was concluded that the best method of delivering carrier gas to the permeation tube flow system was to control the pressure in the chamber with a low pressure regulator and control the flow rates only with the valves which were used to split the flows. Increasing the pressure from 2-6 in of water minimized signal fluctuations due to differences and flow resistance of individual cartridges.

Additional studies were conducted and are described here in order to determine the performance of the permeation system in delivering reproducible and accurate quantities of organic vapors from permeation tubes and the reprodubility of analysis by high resolution gas-liquid chromatography in combination with the cartridge thermal desorption inlet-manifold.

Experimental

Standard curves were prepared for 9 compounds ranging from non-polar to semi-polar. In each case, a minimum of triplicate analysis was performed for each absolute weight of the organic vapor employed. Linear regression analysis was performed on the response of the flame ionization detector vs quantity of the organic vapor which had been delivered from the permeation system to the Tenax GC cartridge.

The previously described thermal desorption inlet-manifold (1-5) was used for recovering the vapors from Tenax GC cartridges (1.5 cm i.d. x 6.0 cm bed length). Thermal desorption was accomplished at 270°C. A Perkin-Elmer 900 gas-liquid chromatograph equipped with flame ionization detection was used. The chromatographic column was a 100 m glass SCOT coated with OV-101 stationary phase (5). The carrier flow was ∿2.5 ml/min, the hydrogen and air flows to the fid were 35 and 225 ml/min, respectively. The thermal desorption time was 5 min and a 2 min hold period followed by temperature programming of the SCOT column from ambient temperature to 240°C at 4°/min was employed.

For linear regression analysis, peak heights were used of the compounds under study and expressed vs quantity of compound loaded on the Tenax GC cartridge.

Results and Discussion

Figures 3-7 present the standard response curves for each of the compounds studied. The variations are a reflection of the combination of: (1) the delivery of the organic vapor from the permeation device to the Tenax GC cartridge; (2) the trapping of the organic vapor by the Tenax GC cartridge; (3) the efficiency of thermal desorption and transfer to the high resolution glass capillary column; (4) the transmission of the organic vapors through the high resolution column; (5) the linear dynamic range of the capacity of the high resolution column coated with OV-101 phase; (6) the specific organic vapor and (7) the linearity and reproducibility of the flame ionization detector to the organic vapor.

The results shown in Figures 3-7 indicate that the technique of delivering non-polar and semi-polar organic vapors from permeation tubes utilizing the previously described permeation device for synthesizing multi-component air/ vapor mixtures can be achieved in a reproducibile and linear fashion. The one exception was methylene chloride in which some non-linearity was observed throughout the concentration range examined. In most cases, it can seen that the variation was less than 5% with the exception occurring at the higher concentrations. Statistical analysis was performed on these data and the R values at the 95% conference level are also shown in these figures.

The linear regression analyses for these compounds in all cases yield a zero x-y intercept. This is important since it is conceivable that for the quantification of many components in a given sample of ambient air will require the use of response factors based on a "one point response curve" since the use of standard curves of this nature will be excessively time consuming and undesirable for quantification of many compounds. Because the x-y intercept is zero in these cases, the feasibility of using relative molar response (RMR) factors is greatly enhanced.

DEVELOPMENT OF SOFTWARE PROGRAMS FOR QUANTIFICATION OF VOLATILE ORGANICS USING HRGC/MS/COMP

Introduction

Since the information which is generated and available from the mass spectrometer is accumulated on a dedicated computer system, it would be

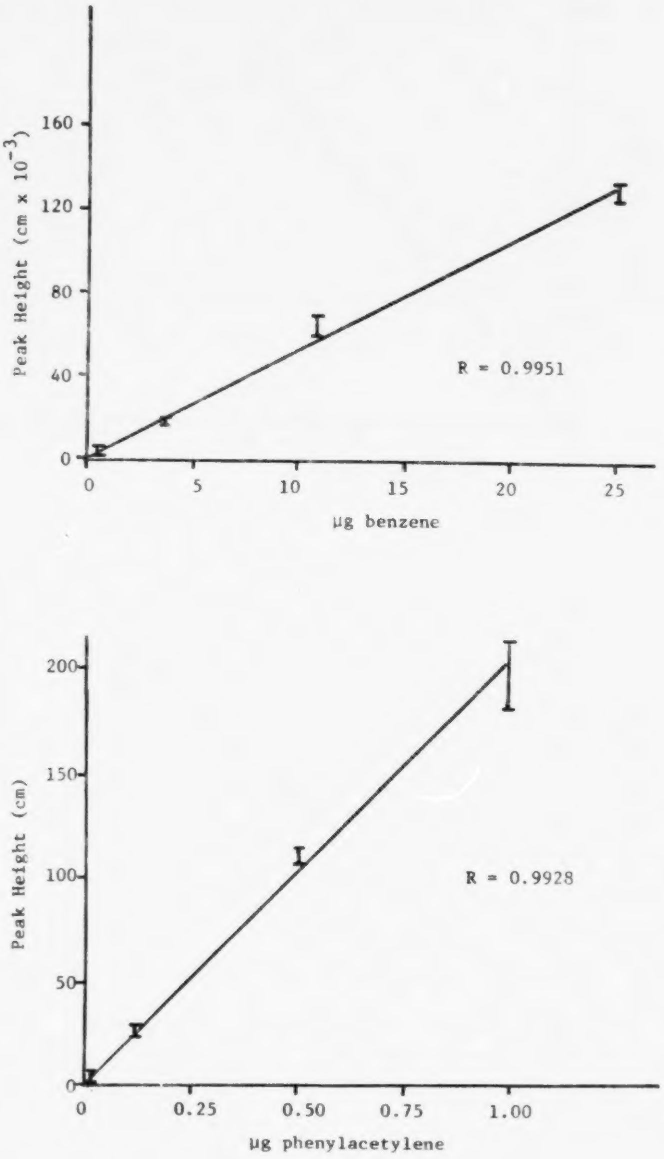


Figure 3. Linear regressions for benzene and phenylacetylene.

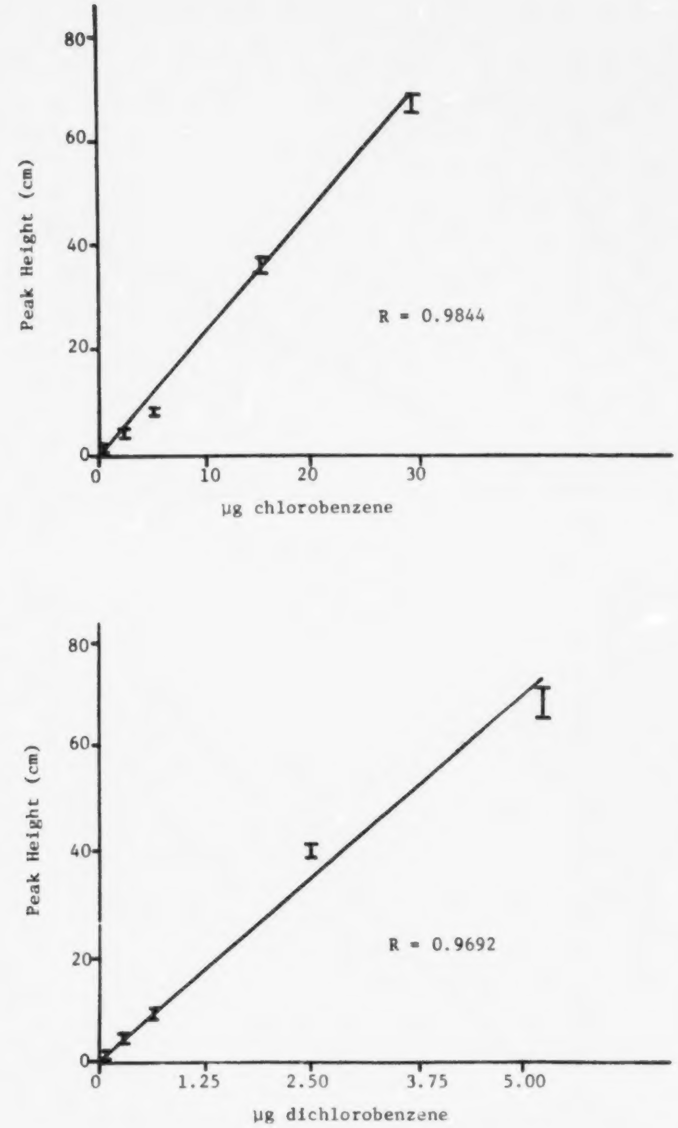


Figure 4. Linear regressions for chlorobenzene and dichlorobenzene.

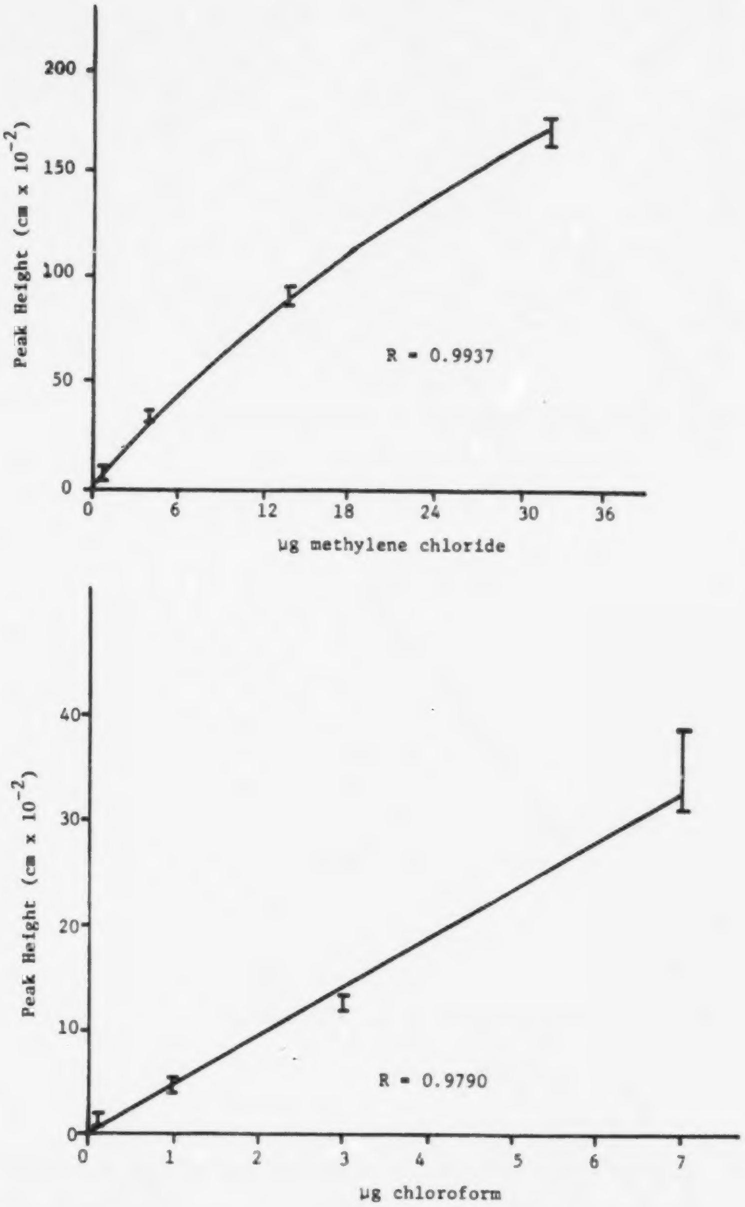


Figure 5. Linear regressions for methylene chloride and chloroform.

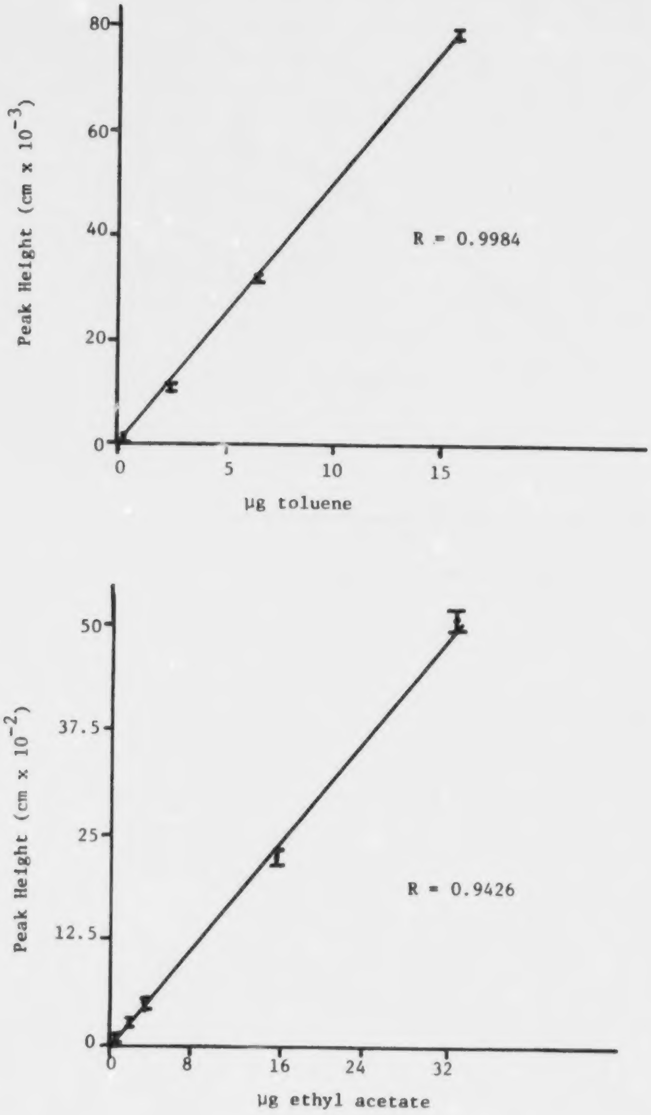


Figure 6. Linear regressions for toluene and ethyl acetate.

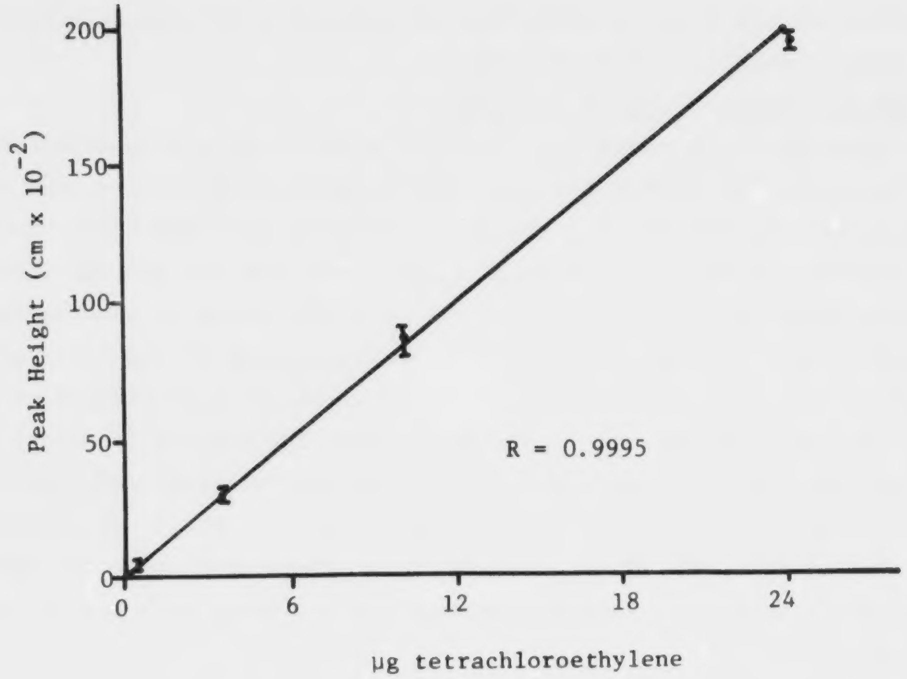


Figure 7. Linear regressions for tetrachloroethylene.

highly desirable to utilize the speed and accuracy of a computer system for the calculation of levels of volatile organic vapors present in the original sample. A previous report (5) described the use of the method of relative molar response factors for quantification of organic vapors in ambient air samples.

This section describes software programs which were fabricated in order to allow the expedient determination of quantities of organic vapors present in samples analyzed by hrgc/ms/comp.

Design of Computer Software Programs

The computer programs were written in BASIC and all quantification was based on mass fragmentography. Two programs were written, one was called "quantiate" and the second "area ratio calculation". The BASIC "quantitate" was designed to search a specified range of spectra for maximum intensity of standard mass and then to search for a different range of spectra for maximum intensity and "unknown" mass followed by calculation of the ratio of their intensities. A printout included maximum intensity for standard mass and spectrum number of maximum intensity and then the maximum intensity for the unknown mass and the spectrum number of maximum intensity and finally the ratio of unknown to standard intensities. Also an option was provided for calculating nanograms of unknown from this information using the RMR factor. The "quantitate" program executed the following mathematical relationships:

$$\mathrm{ng(unknown)} = \frac{R \times M2 \times N1}{M1 \times R1}$$

R = ratio of unknown: standard itensities
M1 = M. Wt. standard
M2 = M. Wt. unknown
N1 = ng standard
R1 = $\mathrm{RMR}_{\mathrm{unk/std}}$

From

$$\mathrm{RMR}_{\mathrm{unk/std}} = \frac{A_{\mathrm{unk}}/\mathrm{moles}_{\mathrm{unk}}}{\mathrm{std}/\mathrm{moles}_{\mathrm{std}}}$$

$$= \frac{A_{\mathrm{unk}}/\mathrm{ng}_{\mathrm{unk}}/\mathrm{m.\ wt}_{\mathrm{unk}}}{A_{\mathrm{std}}/\mathrm{ng}_{\mathrm{std}}/\mathrm{m.\ wt}_{\mathrm{std}}}$$

A = area, or intensity

The "area ratio" program was designed to calculate the area ratio of a selected ion to one specified (or the sum of specified ions up to 8 in number) over a selected range of mass spectra in the gas chromatogram. The program utilized a subroutine for searching spectra stored on the fixed disk. Subsequently the program printed the "sum or ion areas" which was either a specified ion or a series of ions and "selected ion area" as well as the area ratio and then indicated "saturated ion" if any intensity of an ion was $\geq$32,736 (A/D converter saturation point). The program was used to sum ions representing classes of compounds over most of the mass spectra obtained in a gas chromatogram of the individual samples. The m/z 186 ion was used as the "selected ion" since it is representative of the two external standards, perfluorobenzene and perfluorotoluene and the mass spectra corresponding to these two standards was summated. The area measurements were of prime interest in most cases; however the use of "area ratios" was useful for comparison between samples without the use of RMR factors since comparisons could be made in this fashion on a relative basis (e.g. comparison of upwind and downwind across a point source of pollution). Figure 8 depicts the area ratio calculation.

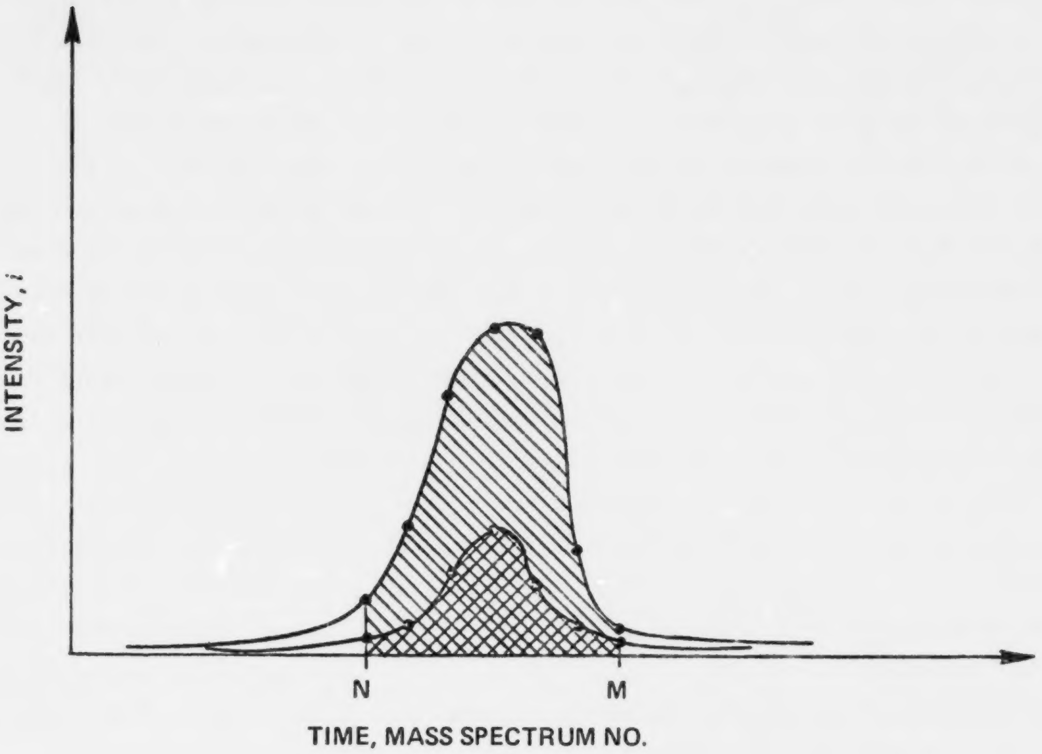
The described computer software programs were written for a 620L computer on a Varian CH-7 mass spectrometer system; however, the principal concept described here was developed as the basis for use in future analysis of ambient air samples whereby quantitative information would be desired for the individual components occurring in the sample.

DETERMINATION OF RELATIVE MOLAR RESPONSE FACTORS (RMR) FOR QUANTIATIVE HRGC/MS/COMP ANALYSIS

Introduction

Described above was the development of computer software programs for quantification of volatile organics by hrgc/ms. These software programs were written in order to expedite the quantification of many organic vapors in air samples.

Because the ambient air samples contain a multitude of organic compounds, it is not feasible to generate standard curves for every single compound for which quantitative information is desired. Instead a relative molar response ratio concept would allow more expeditious estimation of the levels of the



$$\text{Area Ratio} = \frac{\sum_{N}^{M} i_{\text{SELECTED}}}{\sum_{N}^{M} \sum_{1}^{n} i}$$

▧ Sum of ion(s) for specified ion(s)

▨ Selected ion

or

$$\text{Area Ratio } R = \frac{A_2}{A_1}$$

where : A_2 = sum of intensities of selected ion over spectrum range N to M

A_1 = sum of intensities of specified ion(s) over spectrum range N to M

Figure 8. Area Ratio Calculation

components if the method proved to be relatively accurate and reproducibile. Another problem associated with the quantification of many organic vapors occurring in ambient air is that authentic standards are not available for every compound identified. Thus it would be desirable to determine whether empirical correlations could be derived for chemicals within a chemical class in order that extrapolations could be made for substances for which authentic material was unavailable commercially for determining the relative molar response factor. Another objective of this study was to determine the RMR factors for a series of compounds within a chemical class in order to ascertain the sensitivity of the gc/ms/comp system and to assess the possibility of utilizing an average RMR to represent the chemical class and quantification.

Experimental

Table 11 presents the substances which have been selected for RMR determinations. The chemical classes include ketones, aldehydes, alcohols, ethers, esters, nitriles, sulfur compounds, alkanes, aromatics, halogenated aliphatics, and halogenated aromatics.

In order to obtain RMR factors from the hrgc/ms/comp system, synthetic air/vapor mixtures were prepared from a permeation system. Permeation tubes were prepared for a series of compounds listed in Table 10. Six replicate Tenax GC cartridges were simultaneously loaded with the same concentration of 6-8 organic vapors. The general range of the absolute mass used for determining RMR factors were 200-300 ng.

Tenax cartridges were subsequently thermally desorbed and analyzed by hrgc/ms/comp and full mass spectra were acquired. An SE-30 glass SCOT column 100 m in length was used throughout the study. The operating parameters are given in Table 12.

Using the previously described "quantitate" program, the relative molar response factors for each selected ion of the organic compound and the external standards (perfluorobenzene and perfluorotoluene) were calculated. The resulting RMR factor for each replicate cartridge was then subjected to statistical analysis.

Table 11. CHEMICALS SELECTED FOR RMR DETERMINATIONS

Chemical Class	Compound
Ketones	acetone
	methyl ethyl ketone
	methyl vinyl ketone
	2-pentanone
	3-pentanone
	2-heptanone
	3-heptanone
	cyclohexanone
	acetophenone
Aldehydes	acetaldehyde
	acrolein
	2-furaldehyde
	benzaldehyde
	m-tolualdehyde
	phenyl acetaldehyde
Alcohols	1-butanol
	t-butanol
	phenol
Misc. Nitrogenous Compounds	nitromethane
	nitrobenzene
	N,N-dimethylformamide
	pyrrole
	pyridine
	dimethylnitrosamine
	diethylnitrosamine
Sulfur compounds	carbon disulfide
	carbonyl sulfide
Ethers	diethyl ether
	di-n-butyl ether
	tetrahydrofuran
	furan
	2-methylfuran
	2-ethylfuran
	dihydropyran
	cyclohexene oxide
	styrene oxide
	anisole
	benzofuran
	dibenzofuran
	methylbenzofuran
Esters	diethyl fumarate
	diethyl maleate
	ethyl acetate
	methyl methacrylate
Nitriles	acetonitrile
	propionitrile
	butyronitrile
	pentane nitrile
	benzonitrile
Alkanes	n-pentane
	n-hexane
	n-heptane
	n-octane
	n-nonane
	n-decane

(continued)

Table 11 (cont'd)

Chemical Class	Compound	Chemical Class	Compound
Sulfur compounds (cont'd)	2-methylthiophene	Alkanes (cont'd)	n-tridecane
	3-methylthiophene		1-pentene
	thiophene		2-pentene
	2-thiapropane		1-pentyne
	thiacyclohexane		isoprene
	2,3-dithiabutane		isopentane
	2,3-dithiapentane		1-hexene
	3,4-dithiahexane		1-heptene
	benzothiazole		1,3-hexadiene
	2,3-benzothiophene		2-methylhexane
	ethyl methane sulfonate		cyclopentane
	sulfolane		cyclohexane
	dimethyl sulfoxide		cycloheptane
	2-mercaptoethanol		cyclooctatetraene
			cyclohexene
Aromatics	benzene		4-vinylcyclohexene
	toluene		methylcyclopentane
	o-xylene		methylcyclohexane
	m-xylene		
	p-xylene	Halogenated Aliphatics	methylene chloride
	ethylbenzene		chloroform
	o-ethyltoluene		carbon tetrachloride
	m-ethyltoluene		chloroethane
	p-ethyltoluene		1-chloropropane
	1,2,3-trimethylbenzene		2-chloropropane
	1,2,4-trimethylbenzene		1-chlorobutane
	1,3,5-trimethylbenzene		2-chlorobutane
	n-propylbenzene		1-chloropentane
	cumene		2-chloropentane
	2-phenylpropene		3-chloropentane
	phenylactylene		1-chlorohexane

(continued)

Table 11 (cont'd)

Chemical Class	Compound	Chemical Class	Compound
Aromatics (cont'd)	*n*-butylbenzene	Halogenated Aliphatics (cont'd)	1-chloroheptane
	n-pentylbenzene		1-chlorooctane
	styrene		1-chlorononane
	α-methylstyrene		1-chloro-1-butene
	indan		4-chloro-1-butene
	indene		2-chloro-2-butene
	α-pinene		3-chloro-1-butene
			2-chloroethyl ethyl ether
Halogenated Aromatics	bromobenzene		bis-(chloromethyl) ether
	fluorobenzene		1,1-dichloroethane
	chlorobenzene		1,2-dichloroethane
	o-chlorotoluene		1,1-dichloropropane
	m-chlorotoluene		1,2-dichloropropane
	p-chlorotoluene		1,3-dichloropropane
	benzyl chloride		1-bromohexane
	2-chlorostyrene		1-bromoheptane
	3-chlorostyrene		1-bromooctane
	4-chlorostyrene		methylene bromide
			1,1-dibromoethane
			1,2-dibromoethane
			1,1-dibromoethylene
			1,2-dibromoethylene
			1,2-dibromopropane
			1,3-dibromopropane
			bromoform
			1-bromo-2-chloroethane
			bromodichloromethane
			1-chloro-3-bromopropane
			1,2-dibromo-3-chloropropane
			1,1-dichloropropene
			vinylidene chloride
			methallyl chloride

(continued)

Table 11 (cont'd)

Chemical Class	Compound	Chemical Class	Compound
		Halogenated Aliphatics (cont'd)	phosgene
			1,4-dichloro-2-butyne
			trichloroethylene
			1,1,1-trichloroethane
			1,1,2-trichloroethane
			1,1,2-trichloropropane
			1,2,3-trichloropropane
			tetrachloroethylene
			1,1,1,2-tetrachloroethane
			1,1,2,2-tetrachloroethane
			pentachloroethane
			hexachloroethane
			hexachloro-1,3-butadiene
			bromoethane
			bromoethylene
			1-bromoethene
			1-bromopropane
			2-bromopropane
			1-bromobutane
			2-bromobutane
			1-bromopentane
			2-bromopentane
			3-bromopentane
			o-dichlorobenzene
			m-dichlorobenzene
			p-dichlorobenzene
			2,6-dichlorotoluene
			1,2,4-trichlorobenzene
			1,2,3-trichlorobenzene
			1,3,5-trichlorobenzene

Table 12. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold[a]	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC	
100 m glass SCOT-SE/30	25-240°C, 4°C/min
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	*m/e* 20 → 300
scan range, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	6.0
ion source vacuum	~4 x 10^{-6} torr

[a] These analyses utilized an inlet-manifold with a new cryo-heater module- see Ref. 27.

Results and Discussion

An example of statistical data for the RMR factors of chloroform based on m/z 83 and m/z 186 for perfluorobenzene is given in Table 13. Data of this nature was obtained for all the ions selected for all the compounds understudy. As indicated in Table 13, the arithmetic mean for the RMR factor was 0.66 and the standard deviation was ±7.8%.

The RMR factors for several normal alkanes using selected mass ions are listed in Table 14. The selection of several ions for each of the compounds as well as for the external standard assures that quantification can be conducted by mass fragmentography in lieu of complex mixtures being inadequately resolved by the high resolution gas chromatographic column. The selection of ions and use of mass fragmentography provides additional specificity which is not available utilizing total ion current from the mass spectrometer. Since full mass spectra are obtained during the acquisition of data, it was possible to subsequently select an ion representative of the compounds cracking pattern and displaying this *vs* time (mass chromatogram). Since all of this data was automatically acquired during full scanning, the subsequent calculations require simply executing the software programs for determining the relative molar response factors according to the previously described equation.

The RMR factors for several hydrocarbons and aromatic compounds and the statistical deviation obtained for the RMR factors for each of the selected ions is presented in Table 15. As indicated by this data, the deviation is generally <±10% of the determined RMR value. Data obtained by expanding known quantities of the compound into an air space of a glass vessel and the subsequent transfer of an aliquot to a Tenax GC cartridge, was less accurate and reproducible than that obtained from the use of a permeation system.

The RMR factors and statistical deviations for chlorinated hydrocarbons using perfluorobenzene as the internal standard is given in Table 16. For each compound, a series of m/z ions which represent the mass cracking pattern of that compound was selected for determining the RMR with respect to several ions of the internal standard (*e.g.* m/z 186, 117, 167 and 155). This data suggests that for a predominant number of cases the reproducibility for determining RMR's is better than ±10%.

Table 13. STATISTICAL DATA FOR RELATIVE MOLAR RESPONSE FACTOR OF CHLOROFORM BASED ON M/Z 83 and M/Z 186 FOR PERFLUOROBENZENE

Description	Numerical Value
Number of Values (replicates)	6
Arithmetic Mean	0.66
Standard Deviation	0.0518
Sample Variance	0.0022
Estimated True Variance	0.0027
Standard Error of the Mean	0.0211

Table 14. RELATIVE MOLAR RESONSE FACTORS FOR NORMAL ALKANES USING SELECTED MASS IONS

Compound	Ion (m/z)	Perfluorobenzene Ions (m/z)			
		186	117	167	155
n-pentane	43	0.75 ± 0.10	0.97 ± 0.11	4.89 ± 0.99	4.50 ± 0.50
	42	0.53 ± 0.12	0.63 ± 0.10	3.20 ± 0.76	2.99 ± 0.82
	41	0.41 ± 0.07	0.52 ± 0.07	2.64 ± 0.60	2.43 ± 0.67
	57	0.09 ± 0.02	0.12 ± 0.01	0.64 ± 0.14	0.58 ± 0.11
	72	0.09 ± 0.02	0.12 ± 0.02	0.62 ± 0.16	0.57 ± 0.11
n-hexane	57	0.49 ± 0.19	0.64 ± 0.28	3.23 ± 1.45	3.01 ± 1.45
	43	0.42 ± 0.07	0.53 ± 0.24	3.06 ± 0.91	3.26 ± 1.43
	41	0.60 ± 0.13	0.79 ± 0.15	3.98 ± 1.08	3.72 ± 1.26
	56	0.30 ± 0.07	0.39 ± 0.06	2.00 ± 0.61	1.87 ± 0.60
	86	0.16 ± 0.05	0.20 ± 0.06	1.03 ± 0.37	1.48 ± 0.54
n-heptane	43	1.13 ± 0.11	1.43 ± 0.10	7.38 ± 1.29	6.90 ± 0.47
	41	0.74 ± 0.09	0.94 ± 0.07	4.83 ± 0.68	4.52 ± 0.30
	57	0.43 ± 0.02	0.55 ± 0.04	2.85 ± 0.37	2.68 ± 0.44
	71	0.45 ± 0.05	0.58 ± 0.06	3.02 ± 0.55	2.82 ± 0.44
	56	0.29 ± 0.04	0.37 ± 0.05	1.91 ± 0.44	1.80 ± 0.24
	100	0.19 ± 0.02	0.24 ± 0.03	1.28 ± 0.28	1.20 ± 0.20
n-nonane	43	1.71 ± 0.27	2.21 ± 0.48	10.98 ± 2.33	10.28 ± 2.80
	57	1.24 ± 0.24	1.61 ± 0.39	7.80 ± 1.72	7.49 ± 2.29
	85	0.42 ± 0.04	0.55 ± 0.11	2.72 ± 0.50	2.55 ± 0.60
	71	0.32 ± 0.04	0.41 ± 0.03	2.03 ± 0.33	1.77 ± 0.33
	56	0.30 ± 0.02	0.38 ± 0.05	2.39 ± 0.75	1.78 ± 0.35
	42	0.29 ± 0.04	0.37 ± 0.04	1.85 ± 0.29	1.73 ± 0.40
	128	0.23 ± 0.07	0.31 ± 0.02	1.53 ± 0.55	1.43 ± 0.57
n-decane	43	2.99 ± 0.34	3.86 ± 0.30	19.16 ± 2.91	17.74 ± 3.95
	57	2.45 ± 0.38	3.15 ± 0.36	15.74 ± 1.11	14.57 ± 3.78
	71	0.94 ± 0.08	1.21 ± 0.07	6.05 ± 0.85	5.49 ± 0.93
	85	0.53 ± 0.07	0.69 ± 0.07	3.28 ± 0.44	3.10 ± 0.26
	56	0.49 ± 0.09	0.63 ± 0.11	3.12 ± 0.73	2.92 ± 0.89
	42	0.48 ± 0.05	0.62 ± 0.04	3.12 ± 0.48	2.88 ± 0.64
	142	0.30 ± 0.05	0.39 ± 0.04	1.94 ± 0.44	1.73 ± 0.39

Table 15. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR SEVERAL HYDROCARBONS AND AROMATIC USING PERFLUOROBENZENE STANDARD

		m/z 186		117		167		155	
Compound	Ion (m/z)	RMR	SD	RMR	SD	RMR	SD	RMR	SD
n-pentane	43	0.75	0.061	0.97	0.128	4.36	0.473	4.50	0.509
	42	0.52	0.083	0.63	0.025	3.19	0.843	2.97	0.771
	41	0.41	0.049	0.52	0.035	2.62	0.229	2.39	0.371
	57	0.98	0.013	0.12	0.011	0.64	0.047	0.58	0.100
	72	0.08	0.010	0.11	0.0009	0.53	0.054	0.50	0.055
n-hexane	57	0.39	0.085	0.71	0.157	3.05	0.731	2.99	0.895
	43	0.50	0.069	.61	0.116	2.72	0.693	2.88	0.805
	41	0.56	0.007	0.79	0.143	3.46	0.769	3.72	1.030
	56	-	-	0.40	0.094	1.28	0.297	1.19	0.330
	86	-	-	0.20	0.050	0.92	0.282	0.97	0.307
n-heptane	43	1.13	0.127	1.34	0.117	6.47	0.755	6.53	0.105
	41	-	-	-	-	4.07	0.184	4.32	0.091
	57	0.41	0.009	0.54	0.021	2.54	0.115	2.41	0.256
	71	0.41	0.0238	0.54	0.009	2.55	0.134	2.53	0.087
	56	0.29	0.009	0.38	0.009	1.81	0.046	1.64	0.153
	100	0.21	0.006	0.29	0.009	1.32	0.050	1.168	0.023
cyclopentane	42	0.66	0.081	0.75	0.089	5.34	.571	4.76	0.342
	70	0.12	0.015	0.13	0.006	1.07	0.168	0.96	0.125
	55	0.24	0.025	0.27	0.039	1.97	0.548	1.77	0.442
	41	0.22	0.040	0.25	0.050	1.95	0.799	1.97	0.441
n-pentyne	67	0.286	0.033	0.418	0.048	1.995	0.260	1.838	0.176
	53	0.107	0.015	0.147	0.026	0.722	0.133	0.645	0.104
	42	0.064	0.008	0.081	0.008	0.402	0.068	0.360	0.039
	66	0.009	0.0005	0.013	0.001	0.064	0.005	0.058	0.005
benzene	77	0.36	0.009	0.44	0.052	2.88	0.065	2.30	0.133
	52	0.28	0.015	0.37	0.028	2.28	0.009	1.80	0.096
	50	0.25	0.035	0.32	0.033	1.95	0.337	1.62	0.151
	79	0.10	0.021	0.12	0.023	0.78	0.177	0.67	0.160
	74	0.07	0.003	0.09	0.007	0.62	0.010	0.49	0.036
ethylbenzene	91	3.80	0.340	5.07	0.716	29.17	.718	27.72	4.904
	92	0.29	0.025	0.38	0.042	2.26	0.147	2.06	0.289
	106	1.11	0.098	1.51	0.271	8.49	0.659	8.10	1.739
	105	0.16	0.035	0.23	0.032	1.34	0.128	1.24	0.210
	78	0.31	0.006	0.37	0.041	2.21	0.123	2.02	0.290
	77	0.38	0.104	0.52	0.152	2.90	0169	3.04	0.746
o-xylene	91	3.95	1.421	4.77	1.441	25.25	4.36	-	-
	92	0.30	0.096	.36	0.941	2.43	0.97	-	-
	106	1.72	0.596	2.08	0.624	13.96	5.90	-	-
	105	0.73	0.196	0.88	0.168	-	-	-	-
	78	0.27	0.104	.32	0.106	-	-	-	-
	77	0.61	0.193	.73	0.176	-	-	-	-
n-propylbenzene	91	8.00	0.731	9.89	0.337	65.58	11.07	52.77	2.89
	92	0.93	0.111	.14	0.149	.47	1.44	6.00	0.67
	120	1.02	0.040	1.16	0.151	9.07	1.34	7.36	1.09
	105	0.24	0.010	0.27	0.038	2.18	0.23	1.68	0.31
	78	0.27	0.104	0.32	0.106	-	-	-	-
	77	0.61	0.193	.73	0.176	-	-	-	-

(continued)

Table 15 (cont'd)

Compound	Ion (m/z)	m/z 186		117		167		155	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD
phenylacetylene	102	0.69	0.437	0.78	0.499	5.45	2.929	4.85	2.455
	76	-	-	0.25	0.138	1.73	0.786	1.54	0.652
	103	0.06	0.037	0.06	0.041	0.43	0.245	0.39	0.210
	51	0.12	0.048	0.13	0.053	0.91	0.283	0.81	0.231
	74	0.10	0.052	0.11	0.058	0.78	0.335	0.66	0.325
	75	0.08	0.048	0.09	0.056	0.65	0.318	0.55	0.298
cumene	105	2.33	0.931	2.62	1.047	18.32	5.413	16.39	4.381
	120	0.56	0.209	0.64	0.239	4.48	1.230	4.36	0.831
	77	0.47	0.198	0.52	0.225	3.67	1.216	3.30	0.975
	79	0.46	0.206	0.52	0.238	3.61	1.271	3.23	1.047
	106	0.18	0.047	0.20	0.051	1.42	0.285	1.27	0.202
n-butylbenzene	91	2.79	0.577	3.45	0.348	23.01	5.960	18.48	2.903
	92	1.95	1.194	1.68	0.120	2.09	0.080	11.14	0.272
	134	0.58	0.100	0.72	0.051	-	-	3.86	0.499
	105	0.55	0.095	0.68	0.060	4.56	1.183	3.64	1.900
	78	0.26	0.030	0.32	0.006	2.15	0.384	1.73	0.112
benzaldehyde	77	0.57	0.062	0.71	0.021	4.67	0.703	3.77	0.217
	106	0.39	0.019	0.50	0.035	3.28	0.461	2.65	0.110
	105	0.40	0.035	0.50	0.025	3.32	0.554	2.67	0.161
	78	0.09	0.011	0.12	0.020	0.77	0.153	0.62	0.095
	74	0.05	0.003	0.07	0.007	0.43	0.066	0.35	0.030
	51	0.28	0.032	0.35	0.026	2.33	0.478	1.88	0.170
fluorobenzene	96	1.43	0.070	1.71	0.264	11.74	0.563	9.11	1.064
	95	0.13	0.008	0.16	0.020	1.09	0.066	0.86	0.063
	97	0.92	0.005	0.11	0.019	0.73	0.089	0.60	0.069
	70	0.37	0.038	0.46	0.081	3.17	0.052	2.47	0.328
	75	0.11	0.015	-	-	0.94	0.012	0.75	0.081
α-methylstyrene	118	1.205	0.106	1.642	0.217	8.202	1.082	7.305	0.695
	117	1.035	0.105	1.422	0.121	6.710	0.679	6.272	0.582
	78	0.485	0.029	0.682	0.041	3.450	0.361	2.947	0.083
	77	0.390	0.035	0.550	0.042	2.750	0.310	2.375	0.133
	115	0.420	0.034	0.585	0.053	2.915	0.343	2.532	0.212
	50	0.155	0.006	0.202	0.016	1.082	0.138	0.910	0.034

Table 16. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR CHLORINATED HYDROCARBONS USING PERFLUOROBENZENE STANDARD

Compound	ion (m/ℓ)	m/z 186		117		167		155	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD
methylene chloride	49	0.44	0.078	0.62	0.072	4.17	0.818	2.36	0.262
	84	0.33	0.051	0.47	0.062	3.17	0.627	1.79	0.190
	86	0.23	0.044	0.32	0.050	2.16	0.474	1.22	0.151
	51	0.14	0.032	0.21	0.035	1.40	0.346	0.79	0.134
	47	0.07	0.009	0.10	0.009	0.67	0.108	0.37	0.029
	88	0.04	0.006	0.01	0.000	0.36	0.076	0.20	0.025
chloroform	83	0.66	0.052	0.95	0.057	6.01	0.762	3.60	0.095
	85	0.45	0.038	0.62	0.046	4.12	0.460	2.37	0.115
	47	0.20	0.012	0.28	0.015	1.81	0.087	1.01	0.046
	49	0.07	0.009	0.10	0.013	0.68	0.052	0.39	0.057
	87	0.07	0.009	0.10	0.013	0.67	0.113	0.42	0.027
	50	0.03	0.003	0.04	0.005	0.27	0.041	0.16	0.015
carbon tetrachloride	117	0.278	0.053	0.394	0.061	2.307	0.675	1.532	0.274
	119	0.286	0.0416	0.404	0.058	2.280	0.664	1.582	0.266
	121	0.080	0.012	0.113	0.017	0.675	0.179	0.440	0.078
	47	0.047	0.019	0.104	0.024	0.632	0.327	0.406	0.114
	82	0.067	0.019	0.094	0.025	0.508	0.124	0.372	0.122
	49	0.032	0.004	0.045	0.005	0.265	0.029	0.176	0.029
1,2-dichloroethane	62	0.287	0.021	0.382	0.035	2.295	0.204	1.840	0.185
	64	0.085	0.008	0.111	0.012	0.672	0.076	0.530	0.010
	63	0.052	0.007	0.069	0.009	0.400	0.072	0.307	0.030
	61	0.033	0.003	0.044	0.004	0.260	0.042	0.212	0.026
	98	0.037	0.003	0.046	0.001	0.292	0.025	0.207	0.033
	100	0.018	0.004	0.026	0.005	0.155	0.033	0.122	0.026

(continued)

Table 16 (cont'd)

Compound	Ion (m/z)	m/z 186		117		167		155	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD
1,1,1-trichloro-ethane	97	0.550	0.059	0.728	0.102	4.370	0.368	3.586	0.405
	99	0.357	0.025	0.478	0.051	2.770	0.233	2.330	0.099
	117	0.094	0.010	0.117	0.005	0.746	0.089	0.600	0.010
	119	0.089	0.009	0.117	0.016	0.700	0.030	0.577	0.025
	101	0.059	0.005	0.078	0.010	0.470	0.043	0.386	0.034
	60	0.047	0.003	0.062	0.006	0.363	0.021	0.313	0.006
tetrachloro-ethane	166	0.616	0.059	0.766	0.129	3.460	0.479	3.552	0.148
	164	0.502	0.058	0.660	0.101	2.800	0.354	2.717	0.075
	168	0.305	0.037	0.412	0.071	1.734	0.242	1.692	0.023
	129	0.480	0.042	0.680	0.117	2.856	0.340	2.820	0.110
	131	0.470	0.041	0.667	0.095	2.734	0.273	2.710	0.174
	96	0.144	0.018	0.198	0.034	0.842	0.091	0.926	0.022
1,2-dichloro-propane	63	1.342	0.215	1.840	0.074	8.395	0.238	7.590	0.861
	62	1.054	0.135	1.352	0.065	6.178	0.210	6.035	0.796
	65	0.425	0.066	0.557	0.030	2.582	0.100	2.518	0.371
	64	0.348	0.055	0.462	0.029	2.085	0.053	2.060	0.322
	112	0.046	0.008	0.061	0.006	0.283	0.030	0.273	0.048
	114	0.031	0.003	0.040	0.003	0.170	0.014	0.182	0.013
bromodichloro-methane	83	0.543	0.056	0.733	0.061	4.300	0.559	3.536	0.421
	85	0.390	0.018	0.520	0.042	2.970	0.087	2.562	0.065
	87	0.055	0.012	0.077	0.012	0.550	0.046	0.456	0.025
	47	0.123	0.006	0.167	0.006	0.980	0.072	0.830	0.062
	129	0.061	0.007	0.081	0.008	0.480	0.073	0.405	0.068
	127	0.047	0.002	0.062	0.003	0.367	0.022	0.320	0.037

(continued)

Table 16 (cont'd)

Compound	Ion (m/z)	m/z 186		117		167		155	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD
1-bromo-2-chloroethane	63	1.005	0.061	1.387	0.064	6.035	0.391	5.913	0.768
	65	0.317	0.018	0.432	0.019	1.922	0.095	1.870	0.112
	144	0.099	0.007	0.127	0.009	0.607	0.099	0.598	0.030
	142	0.064	0.008	0.091	0.007	0.405	0.024	0.362	0.056
	93	0.036	0.006	0.052	0.005	0.200	0.025	0.214	0.034
	146	0.020	0.003	0.028	0.001	0.123	0.006	0.116	0.018
methylene bromide	93	0.538	0.081	0.760	0.137	4.686	1.302	2.910	0.402
	174	0.582	0.073	-	-	5.126	1.063	3.150	0.355
	95	0.464	0.063	0.562	0.090	4.114	1.174	2.512	0.268
	172	0.310	0.034	0.486	0.049	2.764	0.519	1.700	0.132
	176	0.296	0.035	0.408	0.040	2.660	0.521	1.616	0.119
	91	0.082	0.015	0.113	0.017	0.732	0.208	0.446	0.067
1,2-dibromo-propane	121	1.003	0.078	1.316	0.111	7.927	0.533	7.070	0.764
	123	0.993	0.068	1.300	0.104	7.867	0.495	6.993	0.739
	107	0.039	0.006	0.056	0.008	0.317	0.044	0.250	-
	42	0.150	0.030	0.230	0.017	1.170	0.209	1.130	0.195
	41	1.420	0.026	1.953	0.040	11.363	0.770	8.323	1.106

Table 17 presents RMR factors and statistical deviations for chlorinated aromatics using perfluorobenzene as the internal standard.

Table 18 likewise gives relative molar response factors and standard deviations; however, for several oxygenated compounds using perfluorobenzene as the internal standard. As with the halogenated hydrocarbons, the percent deviation was less than ±10% for each case.

Tables 19-22 also present RMR factors, however the values are calculated with respect to perfluorotoluene as the internal standard using the ions m/z 236, 217, 186, 117 and 167.

This study is the beginning of a long-term study to obtain relative molar response factors for many organic compounds. Data of this nature will be examined to ascertain whether compounds may be selected for the determination of RMR's such that they are represented of their chemical class in order to allow extrapolation to other homologues within a chemical class for which RMR data is not available because of the unavailability of the authentic compound for its determination.

Table 17. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR CHLORINATED AROMATICS USING PERFLUOROBENZENE STANDARD

Compound	Ion (m/z)	m/z 186		117		167		155	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD
chlorobenzene	112	0.962	0.067	1.347	0.142	8.204	1.713	5.026	0.386
	77	0.720	0.072	1.010	-	6.094	1.506	3.696	0.464
	114	0.310	0.018	0.435	0.040	2.640	0.506	1.622	0.105
	74	0.087	0.007	0.120	0.014	0.752	0.150	0.458	0.040
	75	0.076	0.008	0.105	0.006	0.614	0.128	0.394	0.051
	113	0.064	0.029	0.090	0.005	0.560	0.064	0.354	0.029
m-dichlorobenzene	146	1.232	0.178	1.740	0.101	9.853	0.264	8.310	0.637
	148	0.793	0.060	1.053	0.055	6.127	0.446	5.200	0.703
	149	0.056	0.002	0.077	0.003	0.443	0.021	0.363	0.012
	150	0.135	0.006	0.180	0.008	1.033	0.042	0.910	0.065
	111	0.553	0.021	0.743	0.015	4.307	0.257	3.825	0.471
	113	0.173	0.012	0.253	0.021	1.393	0.072	1.173	0.112

Table 18. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR SEVERAL OXYGENATED COMPOUNDS USING PERFLUOROBENZENE STANDARD

		m/z 186		117		167		155	
Compound	Ion (m/z)	RMR	SD	RMR	SD	RMR	SD	RMR	SD
acetone	43	0.672	0.062	0.920	0.083	4.948	0.351	4.134	0.386
	58	0.230	0.023	0.310	0.025	1.747	0.114	1.412	0.132
	42	0.057	0.086	0.079	0.013	0.44	0.035	0.356	0.058
	44	0.019	0.001	0.026	0.004	0.140	0.008	0.116	0.016
ethyl acetate	43	0.683	0.138	0.822	0.134	4.230	0.884	4.426	0.838
	45	0.102	0.018	0.111	0.017	0.567	0.105	0.580	0.129
	61	0.087	0.012	0.097	0.016	0.570	0.104	0.505	0.090
	88	0.023	0.005	0.024	0.006	0.137	0.026	0.125	0.025
methyl ethyl ketone	43	0.502	0.058	0.702	0.065	3.822	0.444	3.115	0.421
	72	0.084	0.011	0.127	0.012	0.694	0.080	0.625	0.069
	44	0.019	0.001	0.027	0.018	0.138	0.008	0.122	0.004
furan	68	0.244	0.025	0.325	0.006	1.832	0.308	1.527	0.189
	40	0.050	0.008	0.067	0.009	0.362	0.076	0.312	0.051
	42	0.092	0.006	0.122	0.011	0.647	0.046	0.565	0.041
	69	0.016	-	0.022	-	0.120	-	0.100	-

Table 19. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR SEVERAL HYDROCARBONS AND AROMATICS USING PERFLUOROTOLUENE STANDARD

Compound	Ion m/z	m/z 236		217		186		117		167	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD	RMR	SD
n-pentane	43	1.20	0.150	1.04	0.021	1.64	0.104	2.41	0.216	5.70	0.300
	42	0.96	0.111	0.65	0.126	1.00	0.021	1.51	0.132	3.58	0.184
	41	0.64	0.088	0.56	0.052	0.95	0.107	1.29	0.081	2.95	0.473
	57	0.17	0.015	0.13	0.056	0.22	0.009	0.29	0.030	0.83	0.015
	72	0.14	0.010	0.12	0.009	0.20	0.014	0.30	0.036	0.73	0.026
n-hexane	57	1.09	0.153	0.83	0.095	1.36	0.168	1.99	0.217	3.99	0.184
	43	0.92	0.055	0.70	0.050	1.15	0.110	1.71	0.301	3.37	0.245
	41	1.19	0.119	0.90	0.081	1.48	0.153	2.17	0.302	4.74	0.407
	56	0.59	0.094	0.45	0.079	0.70	0.147	1.08	0.240	2.15	0.140
	86	0.32	0.021	0.24	0.026	0.40	0.052	0.59	0.145	1.10	0.156
n-heptane	43	1.67	0.106	0.48	0.129	2.59	0.065	3.54	0.295	8.52	0.497
	41	1.03	0.179	0.92	0.021	0.72	0.021	2.53	0.221	6.16	0.328
	57	0.86	0.015	0.49	0.031	0.99	0.044	1.22	0.055	3.49	0.233
	71	0.65	0.025	0.49	0.025	0.96	0.048	1.55	0.089	3.50	0.144
	56	0.47	0.047	.0.40	0.024	0.66	0.021	0.86	0.017	2.10	0.143
	100	0.37	0.04	0.28	0.032	0.51	0.050	0.61	0.077	1.52	0.116
n-octane	43	3.51	0.258	3.20	0.373	4.91	0.556	-	-	16.62	0.965
	41	1.58	0.216	1.23	0.194	2.21	0.541	-	-	7.54	1.224
	57	1.11	0.055	0.86	0.056	0.49	0.239	-	-	5.23	0.631
	85	1.09	0.099	0.85	0.041	0.55	0.135	-	-	5.73	0.680
	56	0.56	0.053	0.44	0.030	0.83	0.117	-	-	3.01	0.466
	71	0.63	0.114	0.49	0.059	0.91	0.096	1.16	0.144	3.35	0.764
	114	0.37	0.017	0.29	0.096	-	-	0.73	0.064	2.05	0.314
n-nonane	43	2.95	0.546	1.86	0.295	3.32	0.271	4.21	0.106	11.52	1.989
	57	2.59	0.311	-	-	2.39	0.292	3.03	0.225	8.24	1.079
	85	0.73	0.085	0.52	0.107	0.85	0.064	1.09	0.031	3.41	0.428
	71	0.53	0.058	0.41	0.050	0.65	0.025	0.82	0.023	2.50	0.144
	42	0.43	0.042	0.33	0.015	0.59	0.021	0.76	0.067	2.54	0.117
	128	0.43	0.195	0.34	0.005	0.80	0.019	0.79	0.066	1.84	0.409
n-decane	43	5.03	0.224	3.64	0.176	7.23	0.185	8.37	1.300	-	-
	57	4.17	0.248	3.23	0.131	5.93	0.229	9.01	0.810	-	-
	71	1.47	0.009	1.17	0.038	2.19	0.040	2.88	0.317	-	-
	85	-	-	0.65	0.046	1.28	0.035	2.07	0.279	-	-
	56	0.81	0.044	0.63	0.055	1.17	0.165	1.88	0.336	-	-
	42	0.83	0.045	0.63	0.010	1.04	0.035	1.76	0.140	-	-
	142	0.51	0.021	0.41	0.015	0.65	0.047	-	-	-	-
cyclopentane	42	0.85	0.093	0.60	0.132	0.87	0.180	1.18	0.081	3.59	0.410
	70	0.17	0.026	0.12	0.036	0.18	0.055	0.24	0.042	0.62	0.201
	55	0.31	0.060	0.22	0.080	0.38	0.129	0.44	0.108	1.39	0.245
	41	0.29	0.062	0.20	0.077	0.31	0.134	0.41	0.124	1.24	0.382
n-pentyne	67	0.306	0.029	0.117	0.018	0.059	0.009	0.009	0.001	-	-
	53	0.218	0.019	0.083	0.011	0.043	0.007	0.007	0.000	-	-
	42	0.360	0.028	0.128	0.09	0.069	0.010	0.011	0.001	-	-
	66	0.602	0.034	0.222	0.022	0.122	0.012	0.019	0.001	-	-
benzene	78	1.93	0.081	0.41	0.025	2.19	0.045	3.59	0.458	8.93	0.683
	77	0.45	0.010	0.33	0.006	0.51	0.000	0.91	0.159	2.08	0.146
	52	0.36	0.035	0.27	0.015	0.41	0.030	0.67	0.044	1.84	0.377
	50	0.38	0.017	0.25	0.026	0.41	0.074	0.65	0.071	1.82	0.112
	79	0.14	0.018	0.10	0.015	0.16	0.028	0.26	0.063	0.62	0.056
	74	0.11	0.013	0.07	0.002	0.11	0.006	0.19	0.030	0.46	0.040

(continued)

Table 19 (cont'd)

Compound	Ion m/z	m/z 236		217		186		117		167	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD	RMR	SD
ethyl benzene	91	5.48	0.469	2.62	0.189	6.80	0.640	8.71	0.802	23.37	0.961
	92	0.42	0.025	0.20	0.010	0.51	0.046	0.66	0.046	1.66	0.170
	106	1.65	0.175	0.78	0.072	2.06	0.226	2.62	0.290	0.49	1.122
	105	0.25	0.026	0.11	0.011	0.31	0.023	0.39	0.051	0.98	0.176
	78	0.39	0.040	0.20	0.025	0.40	0.075	0.63	0.067	1.47	0.273
	77	0.60	0.136	0.26	0.057	0.77	0.021	0.94	0.217	2.37	0.678
o-xylene	91	6.66	1.233	3.77	0.589	0.42	1.302	0.58	1.959	21.24	6.341
	92	0.49	0.081	0.23	0.091	0.55	0.802	0.49	0.078	1.43	0.489
	106	2.90	0.472	1.36	0.512	3.23	0.483	4.79	1.019	8.79	2.389
	105	0.93	0.200	0.53	0.206	1.28	0.201	1.89	0.418	3.43	0.943
	78	0.36	0.106	0.21	0.090	0.67	0.342	0.52	0.178	1.38	0.419
n-propylbenzene	91	10.11	0.387	4.65	0.336	0.89	0.633	16.06	0.653	40.24	1.033
	92	1.51	0.282	0.54	0.079	1.24	0.045	1.83	0.185	4.49	0.199
	120	1.70	0.310	0.83	0.205	0.52	0.190	2.25	0.436	5.51	0.715
	105	0.33	0.085	0.20	0.500	0.35	0.061	0.52	0.125	1.27	0.229
	78	0.56	0.110	0.33	0.085	0.56	0.134	0.88	0.165	2.16	0.278
phenylacetylene	102	0.83	0.344	0.56	0.144	0.83	0.240	1.17	0.491	3.72	2.180
	76	0.26	0.091	0.18	0.035	0.27	0.056	0.39	0.114	1.18	0.593
	103	0.06	0.030	0.04	0.013	0.05	0.002	0.09	0.040	0.30	0.185
	51	0.14	0.030	0.09	0.007	0.14	0.006	0.19	0.040	0.62	0.225
	74	0.09	0.018	0.08	0.013	0.12	0.023	0.17	0.53	0.54	0.254
	75	0.10	0.036	0.07	0.015	0.09	0.032	0.14	0.049	0.45	0.237
cumene	105	2.89	0.651	2.07	0.287	2.90	0.159	4.03	0.794	12.47	4.314
	120	0.71	0.131	0.48	0.020	0.71	0.039	0.98	0.161	3.05	0.982
	77	0.58	0.140	0.39	0.038	-	-	0.80	0.179	2.50	0.953
	79	0.57	0.161	0.39	0.039	0.57	0.062	0.79	0.202	2.47	0.992
	106	0.22	0.021	0.15	0.011	0.23	0.029	0.31	0.023	0.96	0.228
n-butylbenzene	91	3.54	0.378	2.04	0.741	3.84	0.664	5.62	0.659	-	-
	92	2.14	0.145	1.23	0.410	2.31	0.161	3.41	0.241	8.39	0.537
	134	0.74	0.026	0.42	0.113	0.80	0.085	1.18	0.045	2.90	0.296
	105	0.69	0.035	0.39	0.092	0.75	0.075	1.11	0.047	2.74	0.266
	78	0.32	0.145	0.18	0.044	0.36	0.036	0.53	0.026	1.31	0.118
benzeldehyde	77	0.73	0.057	0.38	0.153	0.79	0.090	1.34	0.764	2.84	0.311
	106	0.59	0.369	0.26	0.088	0.54	0.036	0.81	0.062	1.98	0.092
	105	0.53	0.040	0.27	0.088	0.55	0.021	0.82	0.042	2.01	0.050
	78	0.12	0.017	0.07	0.016	0.13	0.011	0.19	0.032	0.45	0.061
	74	0.07	0.007	0.03	0.012	0.07	0.003	0.10	0.012	0.26	0.010
	51	0.36	0.015	0.16	0.021	0.39	0.015	0.57	0.017	1.41	0.060
fluorobenzene	96	1.84	0.300	0.86	0.145	1.98	0.261	2.93	0.483	0.19	0.942
	95	0.17	0.026	0.08	0.012	0.18	0.025	2.55	0.042	0.67	0.075
	77	0.12	0.021	0.07	0.019	0.13	0.017	0.18	0.033	0.47	0.058
	70	0.50	0.096	0.23	0.044	0.49	0.110	0.75	0.167	1.95	0.335
	75	0.15	0.026	0.07	0.016	0.15	0.029	0.23	0.046	0.55	0.106
α-methyl styrene	118	1.282	0.252	0.970	0.186	1.610	0.242	2.625	0.555	-	-
	117	1.114	0.226	0.842	0.166	1.350	0.276	2.275	0.475	-	-
	78	0.524	0.083	0.398	0.067	0.510	0.098	1.077	0.194	-	-
	77	0.418	0.074	0.320	0.057	0.637	0.111	0.861	0.169	-	-
	115	0.442	0.082	0.338	0.065	0.538	0.100	0.910	0.184	-	-
	50	0.168	0.031	0.120	0.021	0.302	0.043	0.345	0.072	-	-

Table 20. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR METHYLENE CHLORIDE AND CHLOROFORM USING PERFLUOROTOLUENE STANDARD

		m/z 236		217		186		117		167	
Compound	Ion (m/z)	RMR	SD	RMR	SD	RMR	SD	RMR	SD	RMR	SD
methylene chloride	49	0.59	0.140	0.41	0.080	0.67	0.123	1.03	0.155	2.39	0.738
	84	0.45	0.098	0.31	0.049	0.51	0.087	0.78	0.100	1.96	0.390
	86	0.31	0.072	0.21	0.042	0.35	0.064	0.53	0.083	1.34	0.300
	51	0.20	0.057	0.14	0.036	0.23	0.050	0.78	0.100	0.87	0.233
	47	0.09	0.213	0.66	0.010	0.10	0.013	0.16	0.021	0.48	0.140
	88	0.05	0.012	0.03	0.068	0.06	0.011	0.09	0.012	0.22	0.049
chloroform	83	-	-	0.63	0.036	1.01	0.098	1.54	0.098	3.99	0.405
	85	-	-	0.43	0.059	0.69	0.108	1.06	0.143	2.61	0.229
	47	0.27	0.029	0.18	0.037	0.31	0.039	0.47	0.056	1.22	0.213
	49	0.10	0.017	0.07	0.013	0.13	0.057	0.17	0.340	0.44	0.100
	87	0.10	0.013	0.07	0.087	0.11	0.017	0.18	0.028	0.45	0.079
	50	0.04	0.099	0.03	0.004	0.05	0.072	0.07	0.012	0.27	0.243
carbon tetrachloride	117	0.442	0.107	0.312	0.069	0.506	0.129	0.762	0.157	-	-
	119	0.460	0.085	0.326	0.059	0.534	0.095	0.788	0.118	-	-
	121	0.128	0.029	0.085	0.013	0.146	0.030	0.218	0.041	-	-
	47	0.120	0.038	0.084	0.027	0.133	0.044	0.200	0.055	-	-
	82	0.108	0.038	0.076	0.029	0.120	0.041	0.170	0.040	-	-
	49	0.0512	0.007	0.036	0.006	0.059	0.009	0.089	0.014	-	-
1,2-dichloroethane	62	0.390	0.062	0.283	0.025	0.443	0.061	0.697	0.090	-	-
	64	0.107	0.005	0.084	0.001	0.127	0.005	0.220	0.017	-	-
	63	0.073	0.010	0.049	0.005	0.083	0.004	0.132	0.005	-	-
	61	0.047	0.002	0.035	0.001	0.055	0.002	0.089	0.008	-	-
	98	0.049	0.008	0.036	0.003	0.058	0.009	0.092	0.006	-	-
	100	0.027	0.004	0.020	0.004	0.032	0.005	0.051	0.010	-	-

(continued)

Table 20 (cont'd)

Compound	Ion (m/z)	m/z 236		217		186		117		167	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD	RMR	SD
1,1,1-trichloroethane	97	0.803	0.127	0.602	0.055	0.917	0.116	1.550	0.036	-	-
	99	0.555	0.058	0.395	0.021	0.617	0.047	1.065	0.075	-	-
	117	0.146	0.026	0.097	0.009	0.145	0.013	0.245	0.017	-	-
	119	0.130	0.028	0.097	0.012	0.160	0.029	0.247	0.006	-	-
	101	0.083	0.009	0.058	0.003	0.100	0.018	0.172	0.009	-	-
	60	0.076	0.002	0.054	0.009	0.089	0.002	0.133	0.006	-	-
tetrachloroethylene	166	0.890	0.063	0.585	0.049	0.930	0.062	1.406	0.107	-	-
	164	0.640	0.063	0.447	0.039	0.715	0.042	1.802	0.063	-	-
	168	0.398	0.051	0.278	0.033	0.447	0.038	0.670	0.057	-	-
	129	0.682	0.065	0.465	0.035	0.717	0.039	1.106	0.084	-	-
	131	0.646	0.064	0.435	0.029	0.695	0.021	1.046	0.046	-	-
	96	0.190	0.014	0.135	0.010	0.212	0.013	0.318	0.026	-	-
1,2-dichloropropane	63	1.755	0.151	1.227	0.110	1.978	0.142	3.058	0.149	-	-
	62	1.295	0.122	0.905	0.088	1.455	0.114	2.250	0.121	-	-
	65	0.540	0.053	0.377	0.039	0.605	0.055	0.937	0.056	-	-
	64	0.437	0.033	0.310	0.026	0.495	0.031	0.762	0.039	-	-
	112	0.058	0.088	0.042	0.066	0.067	0.009	0.102	0.012	-	-
	114	0.036	0.017	0.025	0.017	0.040	0.003	0.064	0.005	-	-
bromodichloromethane	83	0.817	0.125	0.573	0.045	0.960	0.181	1.527	0.210	-	-
	85	0.590	0.101	0.420	0.051	0.647	0.105	1.120	0.093	-	-
	87	0.093	0.020	0.067	0.012	0.099	0.018	0.200	0.026	-	-
	47	0.183	0.025	0.133	0.011	0.213	0.021	0.356	0.030	-	-
	129	0.090	0.008	0.061	0.002	0.108	0.013	0.177	0.029	-	-

(continued)

Table 20 (cont'd)

Compound	Ion (m/z)	m/z 236		212		186		117		167	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD	RMR	SD
1-bromo-2-chloroethane	63	1.285	0.087	0.900	0.071	1.447	0.109	2.450	0.512	-	-
	65	0.400	0.028	0.285	0.024	0.450	0.031	0.712	0.026	-	-
	144	0.125	0.019	0.086	0.008	0.140	0.017	0.223	0.018	-	-
	142	0.082	0.002	0.056	0.002	0.095	0.009	0.15	0.017	-	-
	93	0.047	0.002	0.032	0.002	0.052	0.005	0.799	0.006	-	-
	146	0.027	0.002	0.018	0.002	0.029	0.003	0.046	0.004	-	-
methylene dibromide	93	0.710	0.108	0.517	0.111	0.806	0.126	1.204	0.105	-	-
	174	0.792	0.077	0.558	0.026	0.910	0.069	1.322	0.092	-	-
	95	0.612	0.105	0.432	0.058	0.696	0.112	1.026	0.051	-	-
	172	0.416	0.054	0.296	0.029	0.484	0.043	0.702	0.038	-	-
	176	0.396	0.048	0.284	0.022	0.460	0.037	0.664	0.048	-	-
	91	0.109	0.021	0.275	0.013	0.122	0.018	0.180	0.019	-	-
1,2-dibromopropane	121	1.730	0.117	1.125	0.154	2.027	0.248	3.190	0.442	-	-
	123	1.710	0.117	1.187	0.042	2.000	0.249	3.153	0.428	-	-
	107	0.064	0.013	0.045	0.009	0.074	0.013	0.108	0.017	-	-
	42	0.273	0.021	0.190	0.026	0.323	0.038	0.507	0.101	-	-
	41	2.337	0.078	1.633	0.136	2.737	0.071	3.345	0.782	-	-

Table 21. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR CHLORINATED AROMATICS USING PERFLUOROTOLUENE STANDARD

Compound	Ion (m/z)	m/z 263		217		186		117	
		RMR	SD	RMR	SD	RMR	SD	RMR	SD
chlorobenzene	112	1.240	0.153	0.874	0.084	1.484	0.123	2.152	0.211
	77	0.914	0.170	0.642	0.102	1.056	0.157	1.484	0.251
	114	0.398	0.042	0.280	0.021	0.464	0.032	0.694	0.055
	74	0.112	0.018	0.079	0.010	0.132	0.013	0.198	0.031
	75	0.098	0.016	0.068	0.011	0.113	0.019	0.168	0.024
	113	0.087	0.008	0.061	0.007	0.101	0.009	0.152	0.018
m-dichlorobenzene	146	1.952	0.176	1.395	0.094	2.285	0.182	3.757	0.269
	148	1.215	0.110	0.872	0.085	1.425	0.099	2.345	0.260
	149	0.087	0.013	0.066	0.011	0.100	0.014	0.167	0.024
	150	0.205	0.021	0.150	0.012	0.237	0.019	0.392	0.034
	111	0.862	0.045	0.617	0.021	1.010	0.066	1.662	0.161
	113	0.285	0.025	0.200	0.022	0.330	0.020	0.547	0.051

Table 22. RELATIVE MOLAR RESPONSE FACTORS AND STATISTICAL DEVIATIONS FOR OXYGENATED COMPOUNDS USING PERFLUOROTOLUENE STANDARD

		m/z 236		217		186		117	
Compound	Ion (m/z)	RMR	SD	RMR	SD	RMR	SD	RMR	SD
acetone	43	0.772	0.051	0.555	0.025	0.857	0.049	1.475	0.118
	58	0.265	0.019	0.192	0.009	0.300	0.008	0.452	0.076
	42	0.062	0.011	0.045	0.007	0.072	0.010	0.122	0.024
	44	0.019	0.001	0.014	0.001	0.023	0.002	0.039	0.005
	59	0.024	-	0.077	-	0.027	-	0.046	-
ethyl acetate	43	0.780	0.117	0.596	0.075	0.946	0.129	1.604	0.278
	45	0.116	0.017	0.083	0.014	0.130	0.025	0.224	0.051
	61	0.097	0.009	0.072	0.009	0.115	0.017	0.194	0.036
	88	0.026	0.005	0.018	0.004	0.029	0.066	0.050	0.012
methyl ethyl ketone	43	0.580	0.053	0.415	0.043	0.628	0.071	1.110	0.109
	72	0.106	0.011	0.074	0.007	0.112	0.012	0.197	0.021
	44	0.022	0.003	0.015	0.001	0.023	0.001	0.041	0.003
furan	68	0.272	0.038	0.198	0.018	0.327	0.026	0.540	0.044
	40	0.058	0.011	0.044	0.006	0.069	0.009	0.113	0.015
	42	0.102	0.009	0.074	0.005	0.115	0.006	0.197	0.005
	69	0.016	-	0.012	-	0.018	-	0.032	-

SECTION 7

IDENTIFICATION AND QUANTIFICATION OF ORGANIC POLLUTANTS IN AMBIENT AIR FROM SEVERAL GEOGRAPHICAL AREAS

INTRODUCTION

Three major geographical areas were selected for study. These included: Plaquemine, Geismar and Baton Rouge, LA; Linden, Deepwater and Camden, NJ; and Philadelphia, PA. The Plaquemine, Geismar and Baton Rouge, LA area was chosen because of the high concentrations of synthetic organic chemical producers and petroleum refining operations located along the Mississippi River. Also reported for these three areas, has been a high incidence of cancer (28,29). Thus, these areas would provide an excellent opportunity for further methods development, identification of possible toxic organic chemicals and formulation of pollution profiles.

The main thrust of this program has been to delineate the strengths and weaknesses of the collection and analysis system for vapor phase organic compounds utilizing the techniques of hrgc/ms/comp. This study was undertaken to determine whether the collection and analysis techniques were capable of analyzing for an assortment of chemical classes - oxygen, nitrogen and sulfur-containing compounds.

For the Plaquemine, Geismar and Baton Rouge, LA area the potential emissions and plant locations were examined (30,31) and it was decided that essentially four sites would be studied. These areas included clusters of chemical producers located at Scotts Bluff just north of Baton Rouge, the downtown complex and the industrial sites near Plaquemine and Geismar which are both down river from Baton Rouge. Table 23 presents the potential emissions from chemical industry in Baton Rouge, LA.

The continuing principal objective for including Linden and Deepwater, NJ in this program was to further validate the collection and analysis method for halogenated, aromatic, oxygenated and nitrogen-containing

Table 23. POTENTIAL EMISSIONS FROM CHEMICAL INDUSTRY IN BATON ROUGE, LA[a]

Chemical	Total Production (mmlb/yr)	Raw Material	Company(s)
chlorodifluoromethane (101)	-	chloroform	ACC[c]
dichlorodifluoromethane (12)	-	carbon tetrachloride	ACC
dichloroetetrafluoroethane (114)	NA	perchloroethylene	ACC
ethylene dichloride	1100	ethylene	ACC, EC
polyethylene resin	460	ethylene	ACC
trichlorofluoromethane (11)	-	-	ACC
1,1,2-trichloro-1,2,2-trifluoroethane (113)	NA	perchloroethylene	ACC
vinyl chloride	480	ethylene dichloride	ACC, EC
ethyl chloride	210	ethylene	EC
methyl chloride	75	methanol	EC
perchloroethylene	100	ethylene dichloride	EC
tetraethyl lead	312	ethyl chloride	EC
1,1,1-trichloroethane	40	1,1-dichloroethane	EC
trichloroethylene	32	ethylene	EC
PVC	144	-	EC
benzene	440	petroleum	EXCC
butadiene	428	ethane, etc.	EXCC, CRCC
_n_-butyl alcohol	NA	-	EXCC

(continued)

Table 23 (cont'd)

Chemical	Total Production (mmlb/yr)	Raw Material	Company(s)
decanol[b]	-	nonene	EXCC
diisodecylphthalate	NA	phthalic anhydride, isodecanol	EXCC
dodecene	100	propane/propylene	EXCC
ethylene	700	ethane, etc.	EXCC
isobutylene	NA	petroleum	EXCC
isodecanol[b]	-	nonene	EXCC
isooctyl alcohol[b]	-	neptene	EXCC
isoprene	10	ethylene by-product	EXCC
isopropanol	680	propylene	EXCC
neopentanoic acid	5.5	isobutylene	EXCC
nonene	300	propane/propylene	EXCC
phthalic anhydride	90	o-xylene	EXCC
propylene resin	320	ethylene	EXCC
toluene	378	petroleum	EXCC, FGC
ethylbenzene	900	benzene	FGC
styrene	800	ethylbenzene	FGC
vinyl toluene	NA	toluene, ethylene	FGC

[a] Data provided by the Louisiana State Air Board.
[b] Involves production of other alcohols also, C_6, C_8, C_9, C_{10}, C_{13}, C_{16}.
[c] ACC = Allied Chemical Corp., EC = Ethyl Corp., EXCC = Exxon Chem. Corp., FGC = Foster-Grant Co. Inc.

hydrocarbons associated with the chemical industry. Table 24 presents some of the potential organic compounds associated with the E. I. DuPont de Nemours Facility (Chambers Works) in Deepwater, NJ. Several halogenated hydrocarbons as well as aromatic and oxygenated compounds were suspected to be potentially present in ambient air. Sampling conducted in Linden, NJ at American Cyanamid Corp. was to determine whether N-nitrosoamines were associated with their pesticides synthesis facility. On-site sampling at the DuPont and American Cyanamid Corp. was conducted with the permission of the two industrial companies.

The major portion of the chemical industry in the Camden-Philadelphia area was located in an area 3 or 4 miles north of the Commodore Barry Bridge along both sides of the Delaware River in Chester, PA and Greenwich Township, NJ. Table 25 presents the representative chemical industry along the Delaware River of the Camden, NJ and Philadephia areas (32). The priority organic vapors which were selected for detection and/or quantification, the ambient air for the Camden-Philadelphia area is given in Table 26.

This section describes the characterization of vapor phase organics and their quantification in ambient air for three major geographical areas within the Continental U.S.

EXPERIMENTAL

The sampling methods and qualitative and quantitative techniques used throughout this program are described and incorporated herein as Appendix A. The procedure described in Appendix A essentially is a composite of the techniques which have been developed under previous EPA contracts for the collection of vapor phase, carcinogenic and toxic organic compounds with their subsequent analysis by hrgc/ms/comp (1-27).

The ambient air sampling protocol for Plaquemine is shown in Table 27. Figures 9 and 10 depict the sampling locations. A water tower off the Bayou Road (Location 1) and a Church tower off of the Thesis Street (Location 2) were utilized for overnight sampling. Personal samplers were placed at these two locations and the winds at that time were out of the north from the industrial site (Fig. 9). The sampler on the church tower was in the better position of the two samplers. On the following day (Tuesday), samplers were placed at the corner of David Street and LA988 (Location 3, Fig.

Table 24. POTENTIAL ORGANIC COMPOUNDS ASSOCIATED WITH E. I. DUPONT DENEMOURS FACILITY (CHAMBERS WORKS), DEEPWATER, NJ[a]

Chemical Class	Compound
Halogenated Hydrocarbons	carbon tetrachloride
	vinylidene chloride
	trichloroethylene
	tetrachloroethylene
	ethylene dichloride
	ethylene dibromide
Aromatics	benzene
	toluene
	o-xylene
Oxygenates	methyl methacrylate
	methyl alcohol
	acetone
	phthalic anhydride
	dimethyltetephthalate
Nitrogenous Compounds	nitrobenzene
	acrylonitrile

[a] Provided by Dr. P. Preuss of the New Jersey State Air Board.

Table 25. REPRESENTATIVE CHEMICAL INDUSTRY ALONG THE DELAWARE RIVER OF THE CAMDEN, NJ AND PHILADELPHIA, PA AREAS

Site No.	Site Identification	Site Location or Description
1	Hercules, Inc.	Neck Rd., Burlington, NJ Chemical Mfg. Emp: 125
2	Rohm Haas	Bristol, PA
3	Tenneco Plastic	Beverly Rd., Burlington, NJ Resins, PVC Emp: 230
4	Rohm Haas	North Philadelphia, PA
5	Overall Philadelphia-Camden view	Betsy Ross Bridge
6	Overall Philadelphia-Camden view	Ben Franklin Bridge
7	Overall Philadelphia view	Between Ben Franklin and Betsy Ross Bridges
8	Overall Philadelphia view	Between Walt Whitman and Ben Franklin Bridges
9	Harshaw Chemical Corp.	Foot of Water Street Gloucester, NJ Industrial Metals Inorganic and Organic Chemicals Emp: 96
10	Texaco Oil	West Deptford, NJ Organic Chemicals
11	Mobil Oil Corp. Paulsboro Refinery	Billingsport Rd. Paulsboro, NJ Petroleum Prod., Lubricating Oils, Waxes Emp: 1365

(continued)

Table 25 (cont'd)

Site No.	Site Identification	Site Location or Description
12	Hercules, Inc.	Market St., Gibbstown, NJ Organic Chemicals Emp: 60
13	E. I. DuPont deNemours & Co., Inc.	Rapauno Ave., Gibbstown, NJ Bulk Chemicals Emp: 850
14	Rollins Corp.	Bridgeport, NJ
15	Monsanto Co.	Bridgeport, NJ
16	B. F. Goodrich-Chemicals Division	Pedricktown, NJ
17	Chester, PA Industrial Area View Sunoco Hercules, Inc. British Petroleum Congoleum Fisher Tank	Commadore Barry Bridge
18	Distant Philadelphia view	Gibbstown - Paulsboro, NJ
19	Distant Philadelphia view	Pittman, NJ

Table 26. PRIORITY ORGANIC VAPORS SELECTED FOR DETECTION AND/OR QUANTIFICATION IN AMBIENT AIR FROM CAMDEN-PHILADELPHIA AREA

Chemical	Chemical
1,2-dichloroethane	dimethylterephthalate
chloroform	1,2-dibromoethane
1,1,1-trichloroethane	1,1,2-trichloroethylene
carbon tetrachloride	1,1-dichloroethylene
benzene	nitrobenzene
o-xylene	acrylonitrile
p-xylene	phthalic anhydride
m-xylene	1,1,2,2-tetrachloroethylene
methylmethacrylate	1-chloro-2,3-epoxypropane

Table 27. AMBIENT AIR SAMPLING PROTOCOL FOR PLAQUEMINE, LA AREA

Sampling Locations	Sampling Time (min)	Volume Sampled (ℓ)	Remarks	
Plaquemine, LA City Water Tower, Bayou Rd (L1)	1363	136	1/31-2/1/77 44°F-49% RH	1437-1320 0°/1-12 mph
St. John Evangelist Church Tower, Church and Main St. (L2)	1330	133	1/31-2/1/77 44°F-49%RH	1540-1350 0°/1-12 mph
LA 988 & Davis St. (L3)	250	439	2/1/77 44°F-47% RH	1255-1705 70°/1-12 mph
50 yd East off LA 1N (L4)	190	289	2/1/77 44°F-47% RH	1430-1740 70°/1-12 mph
East off LA 1 (L5)	190	129	2/1/77 44°F-36% RH	1445-1755 70°/1-12 mph
Off LA 1 (L6)	1095	109	2/1-2/2/77 44°F-36% RH	1600-1015 90°/1-12 mph
Off LA 1 on Ms. Armalline Caillouet Property (L7)	990	99	2/1-2/2/77 43°F-36% RH	1745-1015 90°/1-12 mph
Plaquemine Evergreen Plantation (L8)	275	191	2/2/77 57°F-55% RH	1250-1725 80°/1-3 mph
Plaquemine Evergreen Plantation (L9)	230	202	2/2/77 57°F-61% RH	1325-1715 Variable Winds

Table 27 (cont'd)

Sampling Locations	Sampling Time (min)	Volume Sampled (ℓ)	Remarks
Plaquemine Evergreen Plantation (L10)	150	100	2/2/77 1400-1630 56°F-55% RH 90°/variable
Plaquemine Evergreen Plantation (L11)	1035	103	2/2-2/3/77 1705-1020 45°F-99% RH 90°/variable

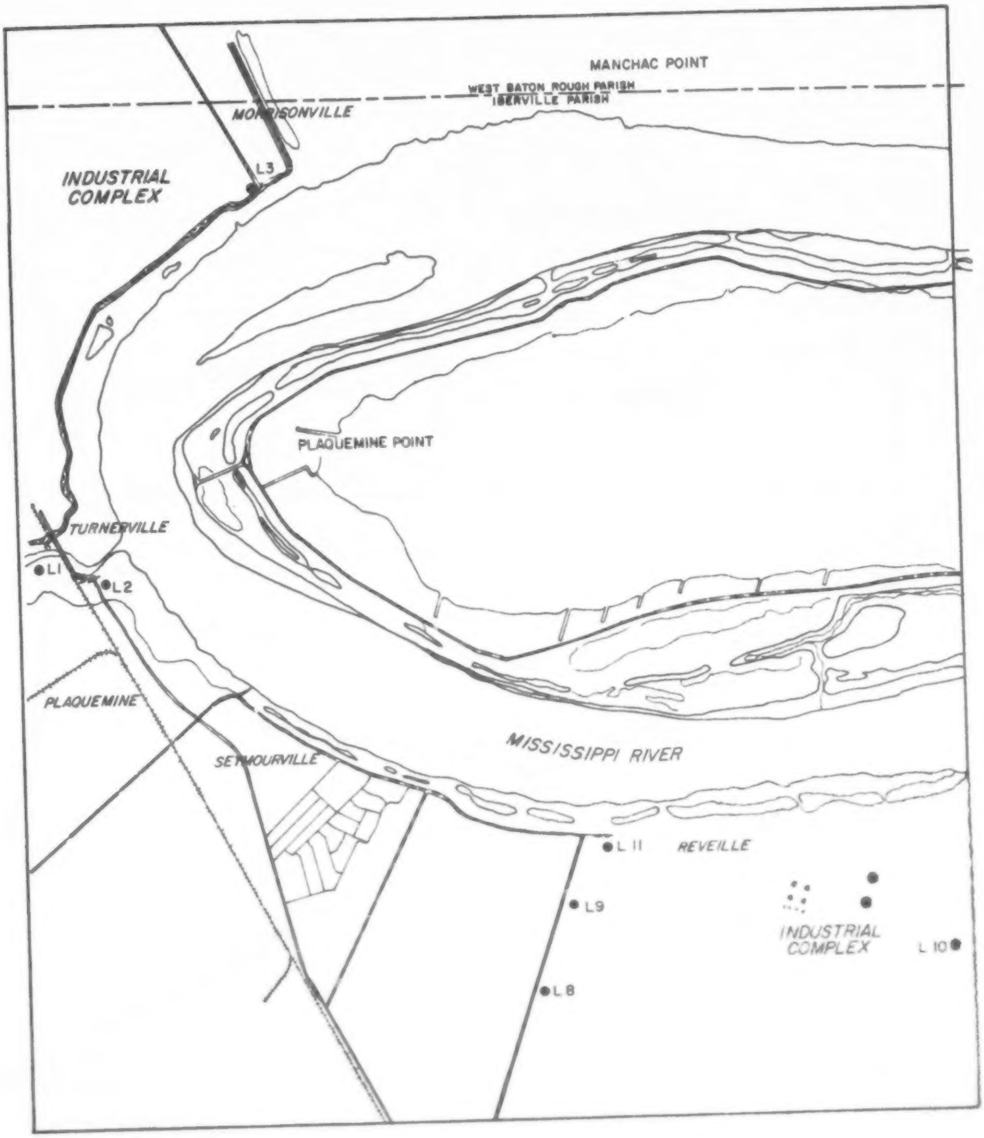

MANCHAC POINT
WEST BATON ROUGH PARISH
IBERVILLE PARISH
MORRISONVILLE
INDUSTRIAL COMPLEX
L3
PLAQUEMINE POINT
TURNERVILLE
L1
L2
PLAQUEMINE
SEYMOURVILLE
MISSISSIPPI RIVER
L 11
REVEILLE
L9
L 8
INDUSTRIAL COMPLEX
L 10

Figure 9. Map depicting locations of ambient air sampling network in Iberville Parish, LA.

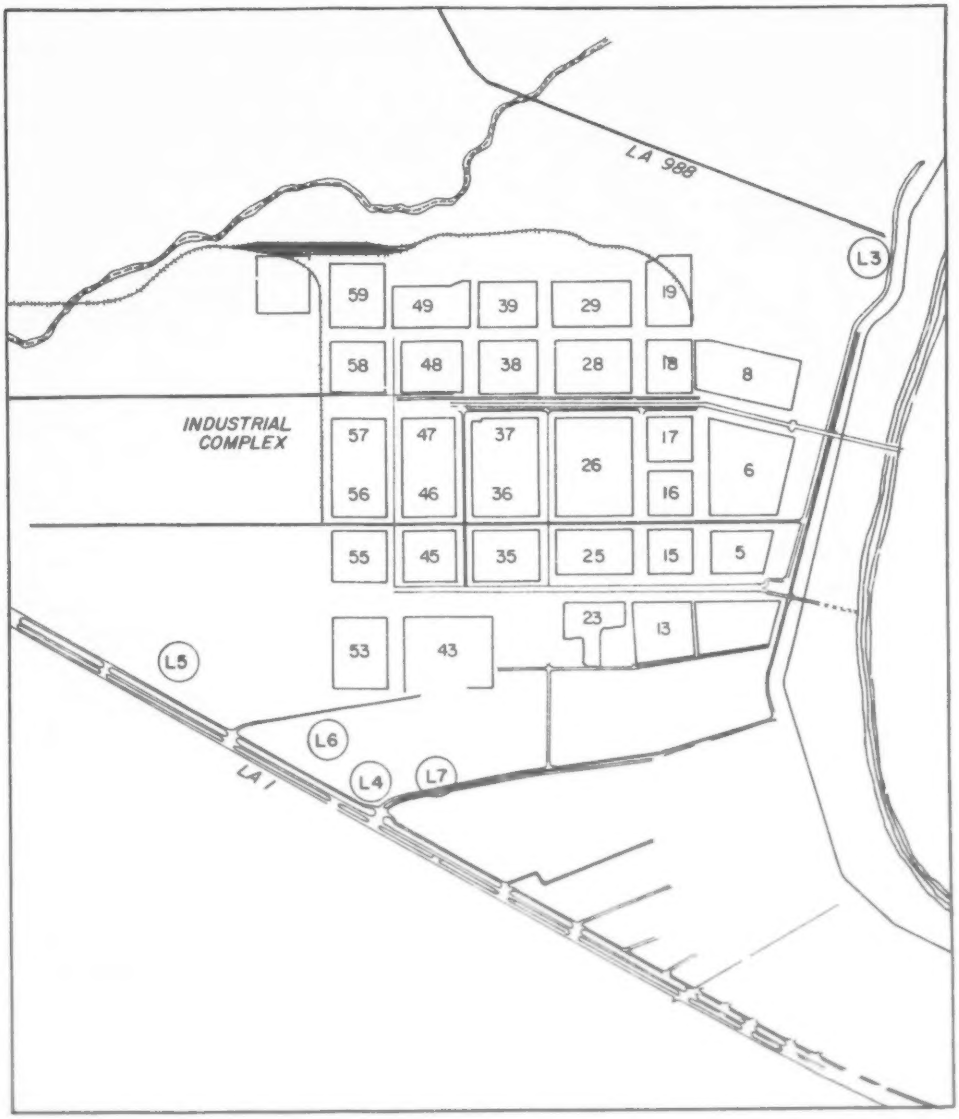

LA 988
L3
59
49
39
29
19
58
48
38
28
18
8
INDUSTRIAL COMPLEX
57
47
37
26
17
6
56
46
36
16
55
45
35
25
15
5
23
13
53
43
L5
L6
L4
L7
LA 1

Figure 10. Map depicting sampling locations near industrial complex in Iberville Parish, LA.

9) which constituted an upwind sample and on the west side of the industrial site (Locations 4 and 7, Fig. 10). Overnight sampling was conducted just west at the industrial site at Location 6 and 7 (Fig. 10). According to the meteorological data, these samplers were in an excellent downwind position from the industrial site. Location 7 was located on private property. On Wednesday, a different industrial area was examined. Samplers were placed downwind on the edge of a sugarcane field off an adjourning road between LA1 and LA405 (Locations 8 and 9, Fig. 9). An upwind sample was taken on a farm at the east side of the industrial area (Location 10). Distinct odors from these plants were detected throughout the entire sampling period. Overnight sampling was conducted under a shed just north of the sugarcane field at Location 11 (Fig. 9). This sampling location representated a good downwind position for only a portion of the sampling period since the winds changed to the north toward the morning hours. A meterological research incorporated weather station was used to provide a continuance readout of wind direction, speed, humidity and temperature at the sampling site (5). Meterological data was also obtained from the local airport. Hand-held instrumentation was also used occassionally to check the performance of the air MRI weather station (5).

Ambient air sampling protocol for Baton Rouge, LA is provided in Table 28. The corresponding sampling locations are presented in Figures 11 and 12. The general sampling strategy was to place at least one sampler in an upwind position with the subsequent location of three or four samplers in an arc downwind from the industrial sites. A key to these plants is given in Table 29.

Table 30 presents the ambient air sampling protocol for Linden and Deepwater, NJ. In both cases a total of three sampling periods were incorporated in the study, one of which involved overnight sampling utilizing personal samplers. The corresponding sampling locations are given in Figures 13 and 14 for American Cyanamid Corp. and Figures 15 and 16 for E. I. DuPont de Nemours site.

Sampling protocols for the Camden-Philadelphia areas are given in Table 31 and the locations are provided on Figure 17.

Table 28. AMBIENT AIR SAMPLING PROTOCOL FOR BATON ROUGE, LA AREA

Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Off U.S. 61 North of Plant A (L17)	1400	140	3/3-3/4/77 ~99% RH	1150-1110 120°/light
Off unpaved, unmarked rd. (L18)	1435	143	3/3-3/4/77 ~99% RH	1135-1130 120°/light
Northwest of Plant A on Mr. Ewell's ranch (L19)	235	156	3/3/77 rain	1220-1615 120°/light
Northwest of Plant A on Mr. Ewell's ranch (L20)	260	184	3/4/77 93% RH	1125-1545 90→120°/4 mph
Off unpaved, unmarked rd. (L21)	30	195	3/4/77 93% RH	1207-1237 90°/4 mph
Eastside of LA 61 (L22)	265	146	3/8/77 49% RH	1205-1630 180°/4 mph
Northwest of Plant A on Mr. Ewell's ranch (L20)	195	129	3/8/77 49% RH	1235-1550 180°/4 mph
Off of Turning Basin Rd. (L23)	1190	119	3/8-3/9/77 50% RH	1625-1215 180°/5 mph
Graveyard Area (L24)	1070	107	3/8-3/9/77 50% RH	1640-1030 180°/5 mph

Table 28 (cont'd)

Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Mengel Rd. (L25)	190	124	3/9/77 54% RH	1330-1640 180°/7 mph
Off LA 61 (L26)	180	121	3/9/77 54% RH	1400-1700 100°/7 mph
Off Mengel Rd. (L27)	1090	109	3/9-3/10/77 54% RH	1650-1100 180°/8-9 mph
Off LA 190 (L28)	1080	108	3/9-3/10/77 54% RH	1715-1115 180°/8-9 mph
Off Mengel Rd. (L25)	190	124	3/9/77 54% RH	1330-1650 100°/7 mph
Off LA 61 (L26)	180	121	3/9/77 54% RH	1400-1700 100°/7 mph
Off Mengel Rd. (L27)	1090	109	3/9-3/10/77 78% RH	1650-1100 180°/8-9 mph
Off LA 61 (L28)	1080	108	3/9-3/10/77 78% RH	1715-1115 180°/8-9 mph
Off Mengel Rd. (L25)	240	162	3/10/77 54% RH	1105-1505 180°/7 mph
Off LA 61 (L26)	250	152	3/10/77 54% RH	1140-1550 180°/7 mph

Table 28 (cont'd)

Sampling Location	Sampling Time (min)	Sampling Volume (ℓ)	Remarks	
Choctow Rd. and Pholox St. (L29)	235	173	3/10/77 54% RH	1215-1610 180°/7 mph
LA 1 and LA 190 (L30)	960	96	3/10-3/11/77 75% RH	1700-0900 100°/6 mph

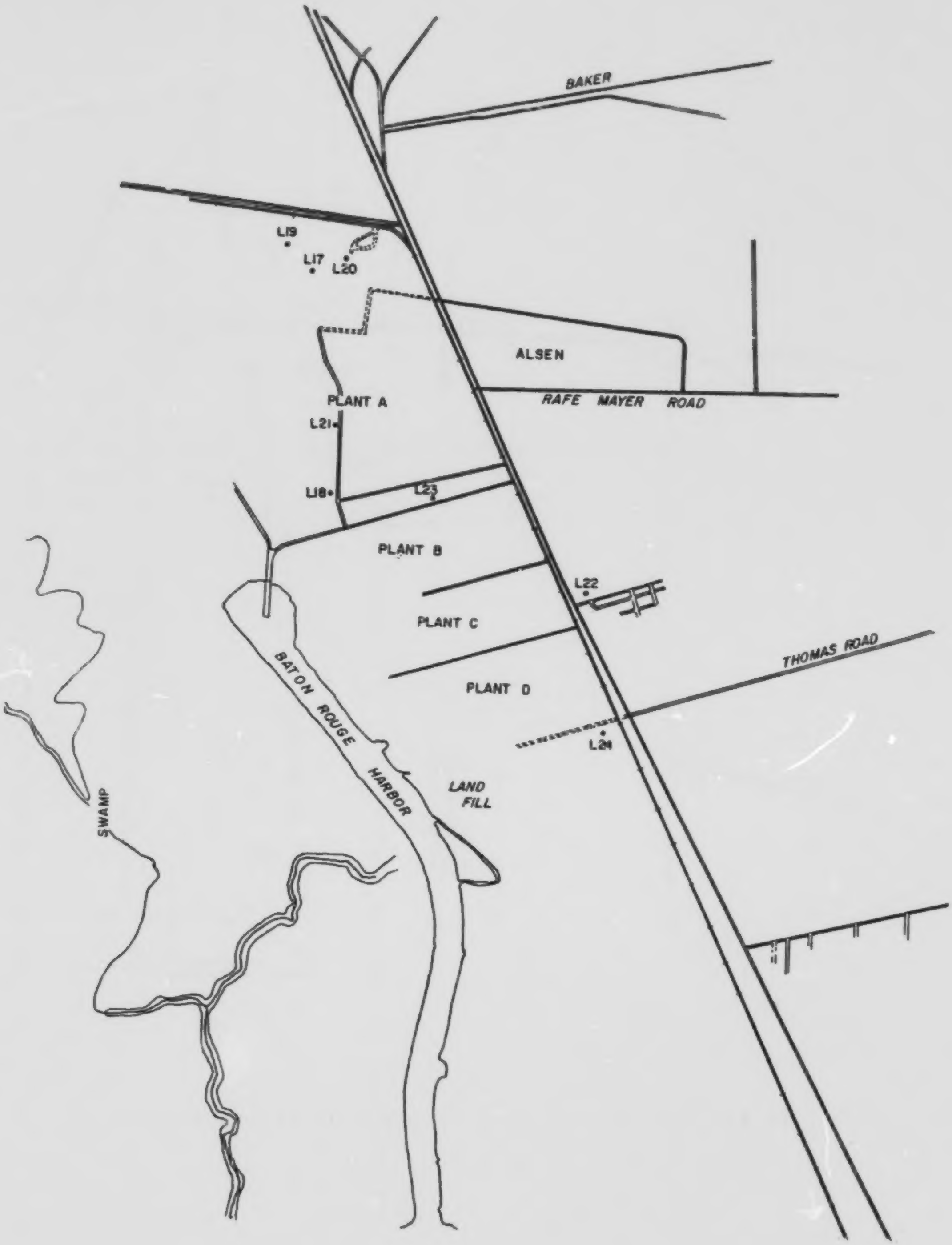

BAKER
L19
L17
L20
ALSEN
RAFE MAYER ROAD
PLANT A
L21
L18
L23
PLANT B
L22
PLANT C
THOMAS ROAD
PLANT D
L24
BATON ROUGE HARBOR
LAND FILL
SWAMP

Figure 11. Sampling site and locations for Baton Rouge, LA Area.

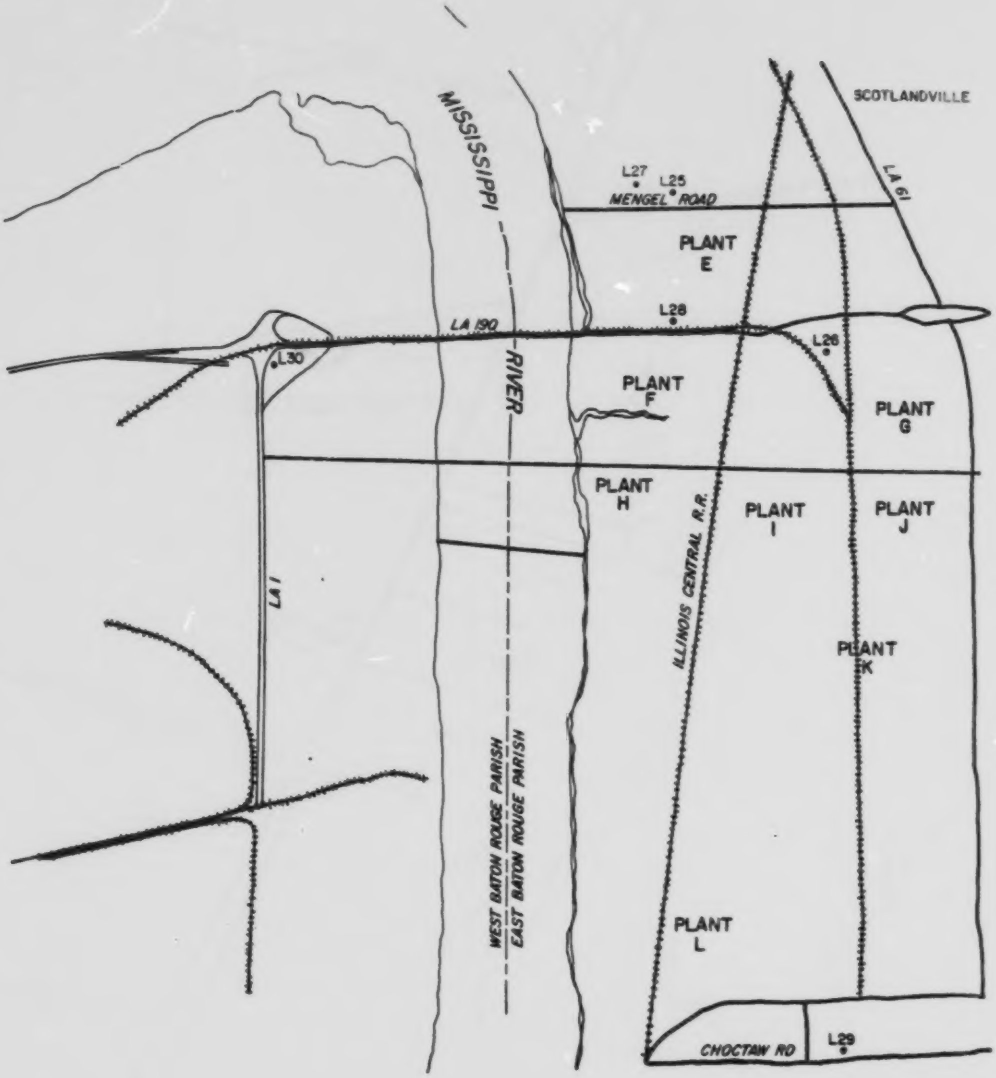

SCOTLANDVILLE
MISSISSIPPI
L27
L25
MENGEL ROAD
LA 61
PLANT E
L28
LA 190
L26
L30
PLANT F
PLANT G
RIVER
PLANT H
PLANT I
PLANT J
ILLINOIS CENTRAL R.R.
LA 1
PLANT K
WEST BATON ROUGE PARISH
EAST BATON ROUGE PARISH
PLANT L
CHOCTAW RD
L29

Figure 12. Sampling site and locations in Baton Rouge, LA.

Table 29. KEY TO MAJOR INDUSTRIAL PLANTS

Plant A - Rollins Environmental Services
Plant B - Allied Chemical Corporation, Plastics Plant
Plant C - Uniroyal Inc.
Plant D - Foster-Grant Co.
Plant E - Stauffer Chemical Co.
Plant F - Kaiser Aluminum & Chemical Corp.
Plant G - Copolymer Rubber & Chemical Co.
Plant H - Allied Chemical North Works, Industrial Chem.
Plant I - Ethyl Corporation
Plant J - Uniroyal Inc., Gulf States Road Plant
Plant K - Exxon USA, refinery
Plant L - Allied Chemical South Works, Specialty Chem.
Plant M - Borden Chemical Company
Plant N - Monochem, Inc.
Plant O - Uniroyal, Inc.
Plant P - Rubicon Chemical, Inc.
Plant Q - BASF Wyandotte Chemical Corp.
Plant R - Shell Chemical Co.
Plant S - Vulcan Materials, Inc.

Table 30. AMBIENT AIR SAMPLING PROTOCOL FOR LINDEN AND DEEPWATER, NJ

Site	Sampling Period/ Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks	
Linden, NJ (American Cyanamid)	P1/L1 (upwind sample)	140	267	6/21/77 48%	76°F 0-30°/10 kts
	P1/L2	137	194	6/21/77 48%	76°F 0-30°/10 kts
	P1/L3	139	228	6/21/77 48%	76°F 0-30°/10 kts
	P1/L4	138	205	6/21/77 48%	76°F 0-30°/10 kts
	P2/L1	1122	101	6/21-22/77 57%	60°F 310°/8-10 kts
	P2/L2	1150	62	6/21-22/77 57%	60°F 310°/8-10 kts
	P2/L3	1145	103	6/21-22/77 57%	60°F 310°/8-10 kts
	P2/L4	1145	103	6/21-22/77 57%	60°F 310°/8-10 kts
	P3/L1	150	236	6/22/77 46%	80°F 330°/1-7 kts
	P3/L2	150	164	6/22/77 46%	80°F 330°/1-7 kts
	P3/L3	150	222	6/22/77 46%	80°F 330°/1-7 kts
	P3/L4	150	202	6/22/77 46%	80°F 330°/1-7 kts

(continued)

Table 30 (cont'd)

Site	Sampling Period/ Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks	
Deepwater, NJ (E. I. DuPont de Nemours)	P4/L5	141	222	6/23/77 53%	79°F 210°/5 kts
	P4/L6	136	147	6/23/77 53%	79°F 210°/5 kts
	P4/L7	127	192	6/23/77 53%	79°F 210°/5 kts
	P4/L8	120	188	6/23/77 53%	79°F 210°/5 kts
	P5/L5	973	87.6	6/23-24/77 56%	58°F 170°/2 kts
	P5/L6	1000	90	6/23-24/77 56%	58°F 170°/2 kts
	P5/L7	1018	55	6/23-24/77 56%	58°F 170°/2 kts
	P5/L8	1040	91.8	6/23-24/77 56%	58°F 170°/2 kts
	P6/L5	120	189	6/24/77 47%	78°F 10°/4 kts
	P6/L6	120	128	6/24/77 47%	78°F 10°/4 kts
	P6/L7	120	172	6/24/77 47%	78°F 10°/4 kts
	P6/L8	120	183	6/24/77 47%	78°F 10°/4 kts

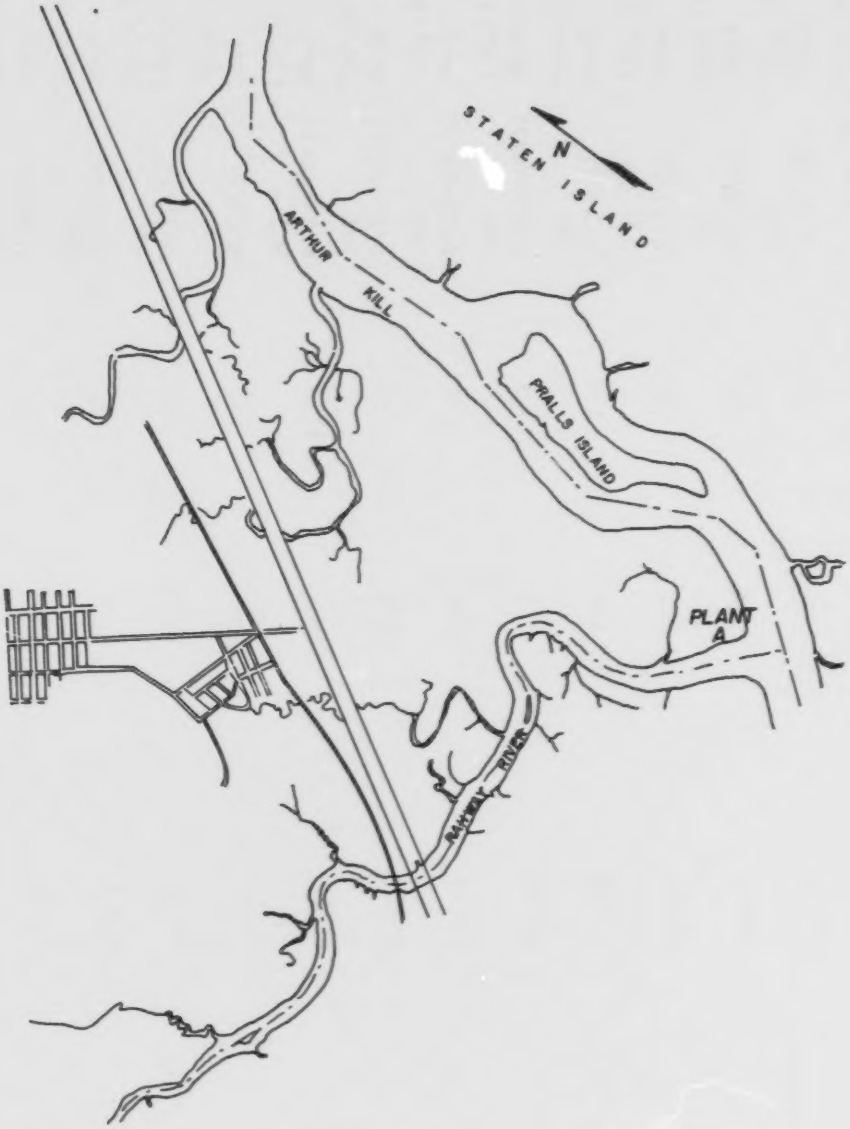

STATEN ISLAND
N
ARTHUR KILL
PRALLS ISLAND
PLANT A
RAHWAY RIVER

Figure 13. General location of American Cyanamid Corp. with respect to Tremley's Point and Staten Island.

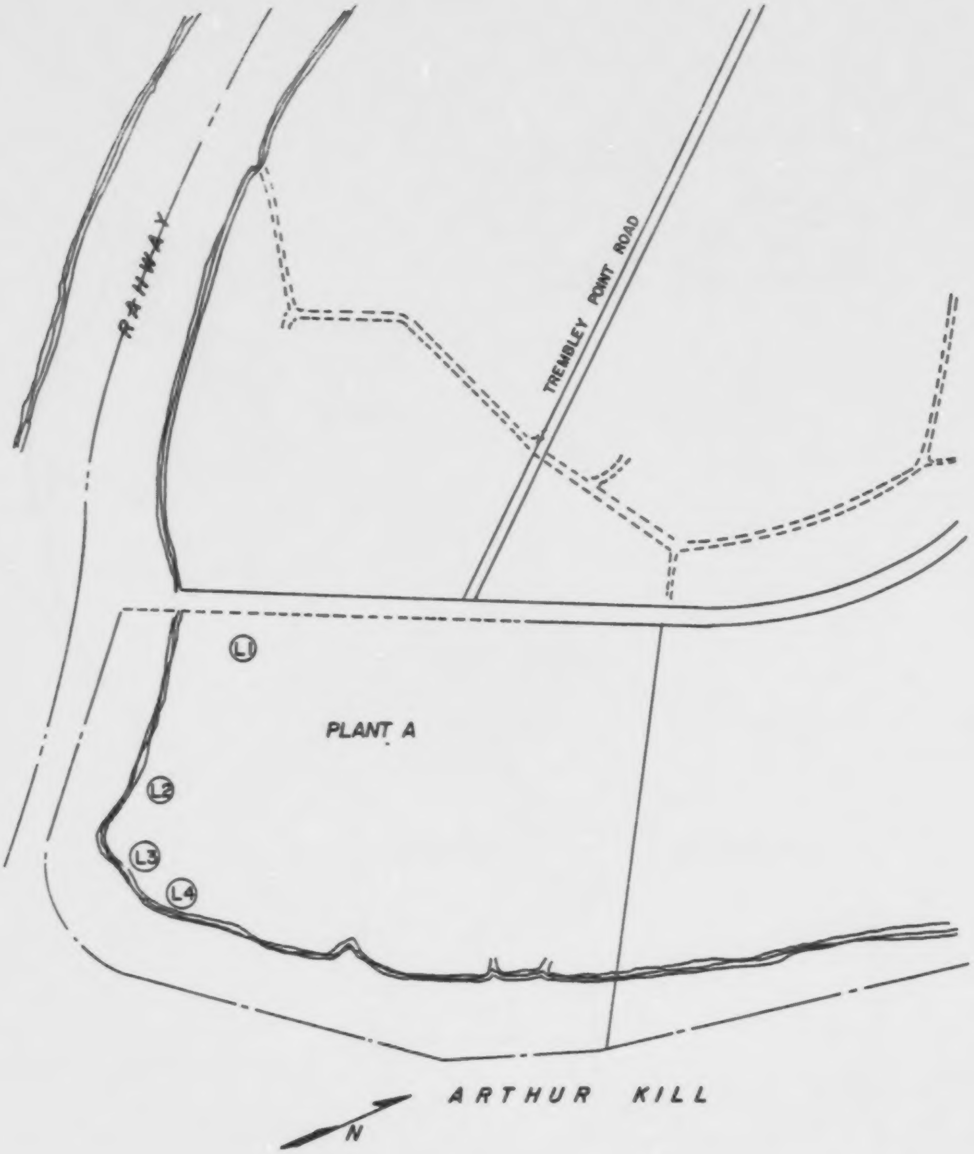
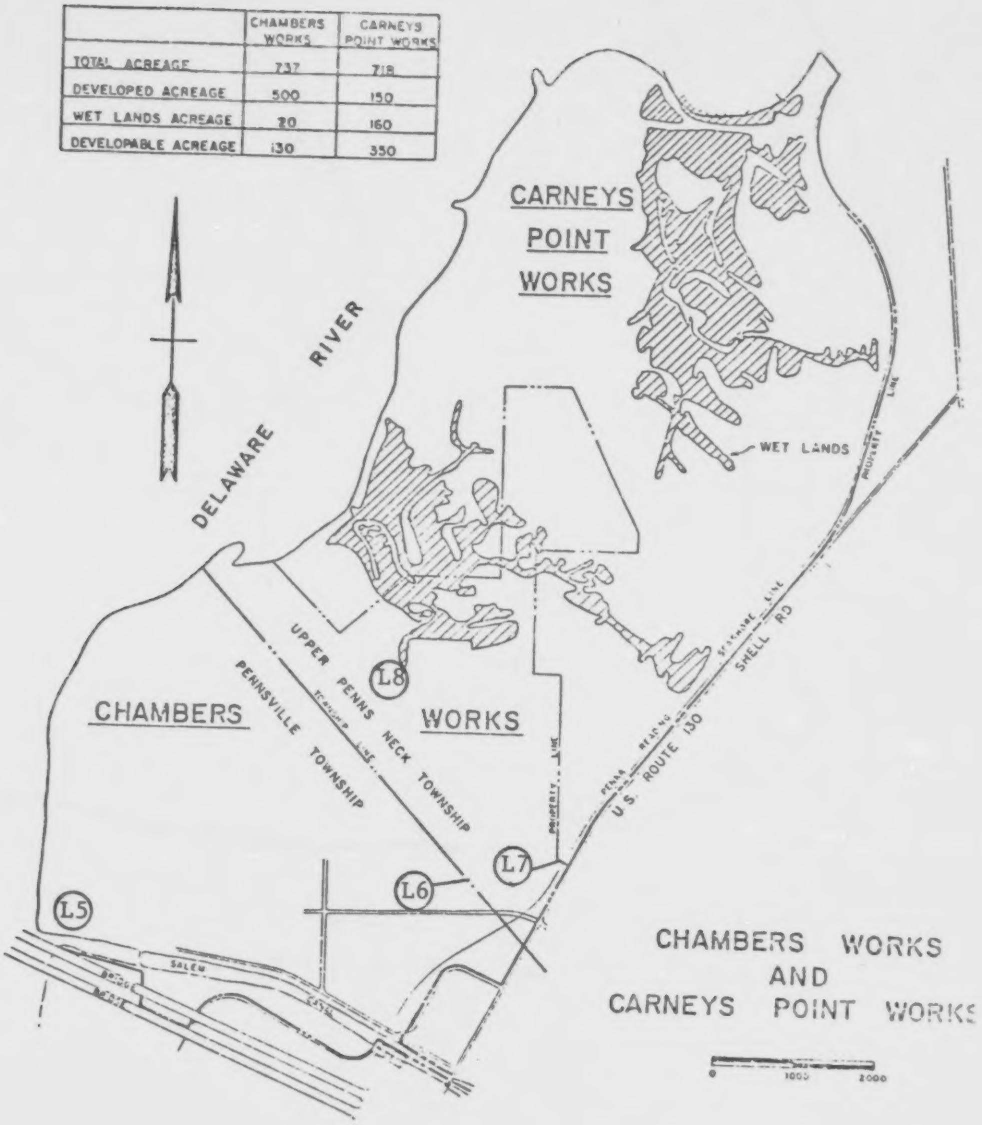

RAHWAY
TREMBLEY POINT ROAD
L1
PLANT A
L2
L3
L4
ARTHUR KILL
N

Figure 14. Sampling locations on American Cyanamid Corp. plant site.



	CHAMBERS WORKS	CARNEYS POINT WORKS
TOTAL ACREAGE	737	718
DEVELOPED ACREAGE	500	150
WET LANDS ACREAGE	20	160
DEVELOPABLE ACREAGE	130	350

CARNEYS POINT WORKS
DELAWARE RIVER
WET LANDS
PROPERTY LINE
CHAMBERS WORKS
UPPER PENNS NECK TOWNSHIP
PENNSVILLE TOWNSHIP
TOWNSHIP LINE
PROPERTY LINE
PENNA READING SEASHORE LINE
U.S. ROUTE 130
SHELL RD
L5
L6
L7
L8
SALEM
CANAL
CHAMBERS WORKS AND CARNEYS POINT WORKS
0
1000
2000

Figure 15. General location of E. I. DuPont de Nemours

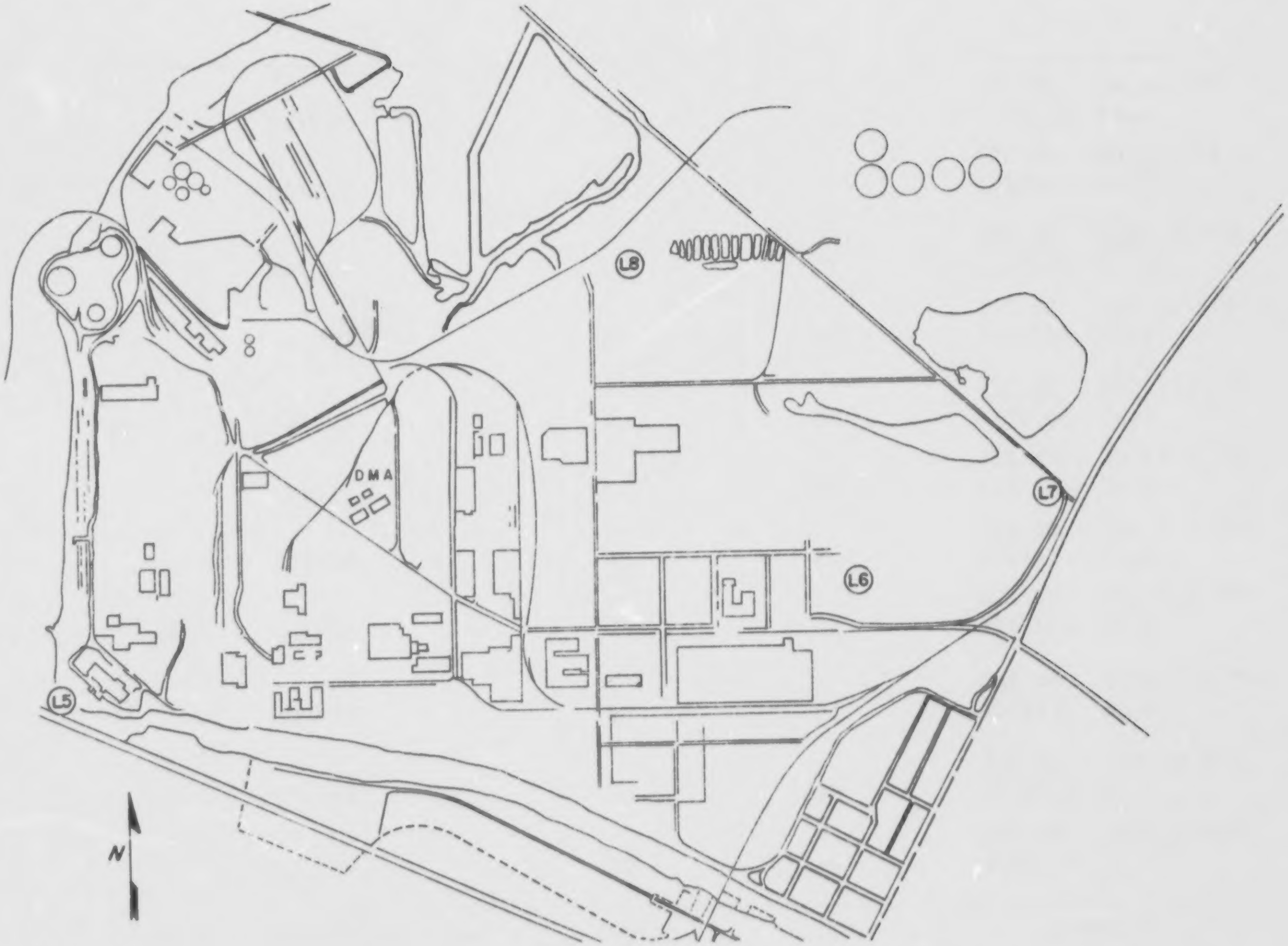

L8
L7
L6
L5
DMA
N

Figure 16. Sampling locations on E. I. DuPont deNemours plant site.

Table 31. AMBIENT AIR SAMPLING PROTOCOL FOR CAMDEN/PHILADELPHIA AREA

Site	Sampling Period/Location	Sampling Time (min)	Volume Sampled (ℓ)	Remarks
Bristol, NJ	P1/L1A	60	55	9/19/77 87°F 52% RH 270°/5 kts
	P1/L1B	60	58	9/19/77 87°F 52% RH 270°/5 kts
Burlington, NJ	P2/L2A	60	54	9/19/77 92°F 53% RH 340°/1-3 kts
North Philadelphia, PA	P3/L3A	60	63	9/21/77 59°F 85% RH 30°/1-3 kts
	P3/L3B	60	54	9/21/77 59°F 85% RH 30°/1-3 kts
	P4/L4A	60	62	9/21/77 59°F 85% RH 30°/1-3 kts
	P4/L4B	60	54	9/21/77 59°F 85% RH 30°/1-3 kts
Markus Hook, NJ	P5/L5A	60	62	9/22/77 62°F 74% RH 100°/5 kts
	P6/L6A	60	55	9/22/77 62°F 74% RH 100°/5 kts
Logan Township, NJ	P7/L7A	60	65	9/22/77 67°F 78% RH 80°/5 kts
	P8/L8A	60	37	9/22/77 69°F 78% RH 75°/5 kts

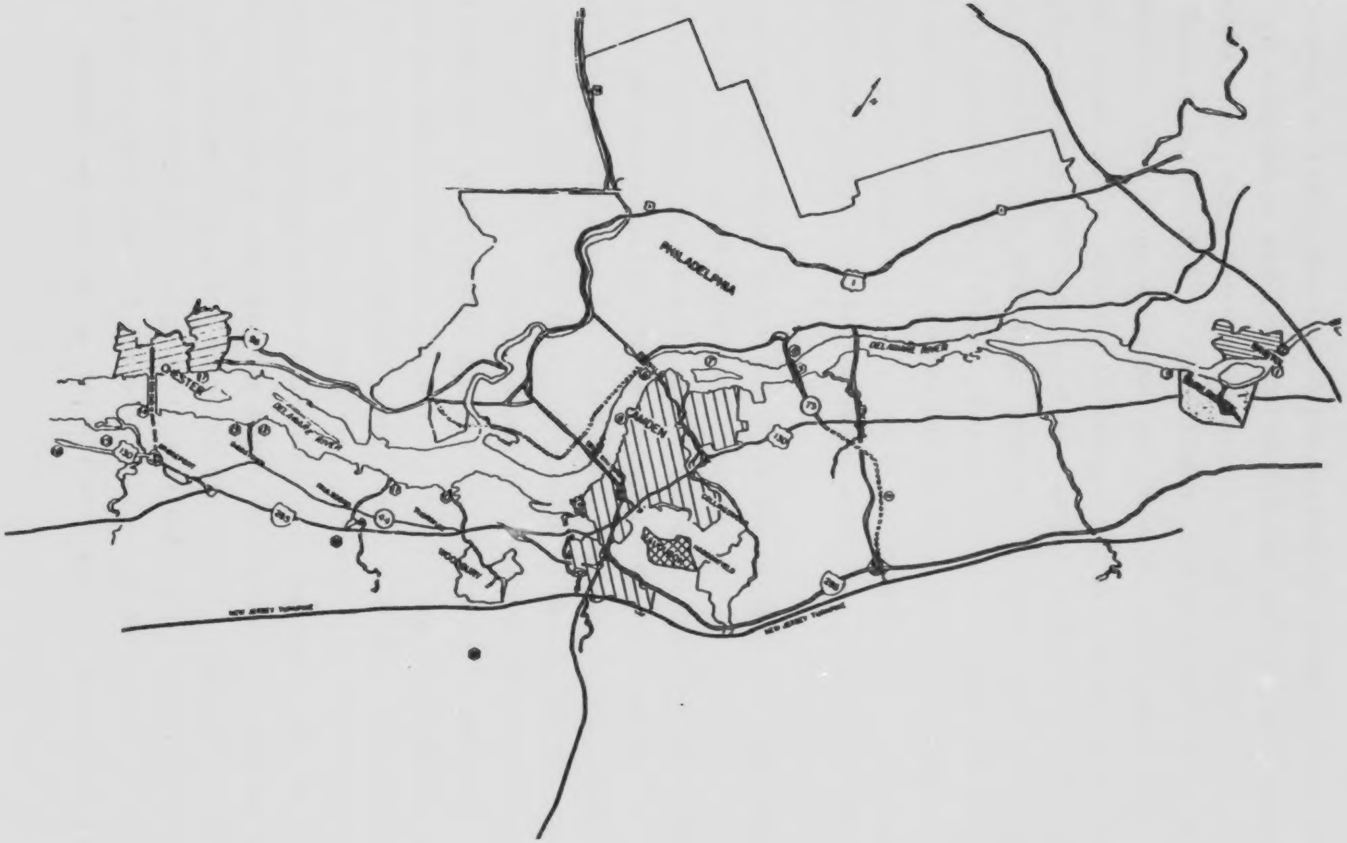

PHILADELPHIA
CAMDEN
CHESTER
DELAWARE RIVER
DELAWARE RIVER
NEW JERSEY TURNPIKE
NEW JERSEY TURNPIKE
1
73
130
295

Figure 17. Map of Chester, Camden, Philadelphia areas along the Delaware River

RESULTS AND DISCUSSION

Plaquemine, Geismar, and Baton Rouge, LA and Vicinity

Qualitative Analysis--

The vapor phase organic pollutants which were identified in several ambient air samples taken from the Plaquemine are given in Appendix B. Table 32 lists the summary of the volatile halogenated organics in ambient air which were identified from this sampling site. Over 30 halogenated hydrocarbons were identified. Many of the compounds which were characterized appeared to be site-specific to the industrial complex, particularly for those samples which were taken at downwind locations. The probable site-specific pollutants were: chloroacetylene, vinyl chloride, chloroethane, vinylidene chloride, dichloropropene isomers, 1,1,2-trichloroethane, bis-(2-chloroisopropyl)ether, tetrachlorobutadiene isomers, 1,3-hexachlorobutadiene, 1,3-dichloropropane, trichloropropene isomers, 1,1,2,2-tetrachloroethane, tetrachloropropane, pentachloroethane, hexachloroethane, pentachlorobutadiene and chlorotoluene isomers.

A selected number of samples (8) were thoroughly characterized for all oganic pollutants present in the ambient air of Baton Rouge, LA. These results are given in Appendix B. Samples were chosen for complete interpretation based on the most favorable meteorological conditions during sampling which would potentially yield the largest number of compounds and the highest concentrations. Tables B1-B16 in Appendix B provide a detailed listing of organic vapors which were identified in these samples.

Table 33 presents a summary of the organic vapors which were identified in ambient air in Baton Rouge, LA. A total of 18 halogenated hydrocarbons and 25 oxygenated compounds were identified. The downwind positions from various industrial sites were given by locations nos. 21, 26 and 27. In these samples, two new compounds were identified which had not been previously determined in ambient air samples collected and analyzed by the described technique. These compounds were β-chlorostyrene and a chloroprene dimer. Chloroprene had been previously identified in samples from Milby Park in Deer Park, TX (4). Furthermore, we have detected 1,3-hexachlorobutadiene which was also present in samples from Plaquemine, LA and the Houston, TX

Table 32. SUMMARY OF VOLATILE HALOGENATED ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH IN LOUISIANA

Compound	Location[a]							
	L2	L4	L5	L6	L7	L8	L9	L11
Dichlorodifluoromethane	+[b]	-[c]	-	-	-	-	-	-
Trichlorofluoromethane	+	-	-	-	-	-	-	-
Methylene chloride	+	+	+	+	+	+	+	-
Chloroform	+	+	+	+	+	+	+	+
1,1,1-Trichloroethane	+	+	+	+	+	+	+	+
1,2-Dichloroethane	+	+	+	+	+	+	-	-
Carbon tetrachloride	+	+	+	+	+	+	+	+
Dichlorobutane isomer	+	-	-	-	-	-	-	-
Tetrachloroethylene	+	+	+	+	+	+	+	+
1,2-Dichloropropane	-	+	+	+	+	-	-	-
Trichloroethylene	-	-	+	+	+	+	+	+
Chloroacetylene	-	-	-	+	-	-	-	-
Vinyl chloride	-	-	-	+	+	+	-	-
Chloroethane	-	-	-	+	+	-	-	-
Vinylidene chloride	-	-	-	+	+	-	-	-
1,1-Dichloroethane	-	-	-	+	+	-	-	-
Dichloropropene isomer(s)	-	-	-	+	+	-	-	-
1,1,2-Trichloroethane	-	-	-	+	+	-	-	-
Dichlorobenzene isomer(s)	-	-	-	+	+	+	-	-
Bis-(2-chloroisopropyl)ether	-	-	-	+	+	-	-	-
Tetrachlorobutadiene isomer(s)	-	-	-	+	+	-	-	-

Table 32 (cont'd)

Compound	Location							
	L2	L4	L5	L6	L7	L8	L9	L11
1,3-Hexachlorobutadiene	–	–	–	+	+	–	–	–
1,3-Dichloropropane (tent.)	–	–	–	–	+	–	–	–
Trichloropropene isomer(s)	–	–	–	–	++[d]	–	–	–
1,1,2,2-Tetrachloroethane	–	–	–	–	+	–	–	–
Tetrachloropropane	–	–	–	–	+	–	–	–
Pentachloroethane	–	–	–	–	+	–	–	–
Hexachloroethane	–	–	–	–	+	–	–	–
Pentachlorobutadiene (tent.)	–	–	–	–	+	–	–	–
Chlorobenzene	–	–	–	–	–	+	–	–
Chlorotoluene isomer(s) (tent.)	–	–	–	–	–	+	–	–

[a] See Table 27 and Fig. 11 and 12 for protocol and sampling locations.

[b] + = detected

[c] – = not detected

[d] more than one isomer detected

Table 33. SUMMARY OF ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR IN BATON ROUGE, LA AND VICINITY

Chemical Class	Compound	Sampling Locations[a]							
		L-17	L-21	L-23	L-26	L-27	L-28	L-30	L-26A
Halogenated hydrocarbons	chloromethane	–[b]	+	–	–	–	–	–	–
	dichloromethane	+	+	+	+	+	+	+	+
	chloroform	+	+	+	+	+	+	+	–
	chloroprene	–	+	–	–	–	–	–	–
	1,1,1-trichloroethane	+	+	+	–	+	–	+	–
	1,2-dichloroethane	+	–	+	+	+	+	+	+
	carbon tetrachloride	+	+	+	+	+	+	+	+
	trichloroethylene	+	+	+	–	–	–	–	+
	tetrachloroethylene	+	+	+	–	+	+	–	+
	2,3-dichlorobutane (tent.)	–	+	–	–	–	–	–	–
	1,2-dichlorobutane (tent.)	–	+	–	–	–	–	–	–
	1,1,2-trichloroethane	–	–	–	–	–	–	–	+
	β-chlorostyrene	–	+	–	–	–	–	–	–
	dichlorobenzene isomer	–	–	+	–	–	–	+	–
	1,1,1,2-tetrachloroethane	–	–	–	–	–	–	–	+
	chloroprene dimer	–	+	–	–	–	–	–	–
	chlorohydrocarbon (unknown)	–	+	–	–	–	–	–	–
	1,3-hexachlorobutadiene	–	–	–	+	–	–	–	+
Oxygenated compounds	acetaldehyde	+	+	+	+	+	+	+	+
	propranol	+	+	–	+	+	+	–	–
	propenal	+	+	–	+	+	+	–	–
	acetone (tent.)	+	+	+	+	–	+	–	–
	n-heptanal	+	–	–	–	–	–	–	–
	benzaldehyde	+	+	+	+	+	+	+	+
	phenol	+	+	+	+	–	+	–	–
	acetophenone	+	+	+	+	+	+	+	–
	n-nonanal	+	+	–	–	+	+	–	+
	cresol isomer	+	+	+	+	+	+	–	+
	n-decanal	+	+	+	–	+	+	–	+
	diethyl ether	–	+	–	–	–	–	–	–
	dimethyl ether	–	+	–	+	–	–	–	–

Table 33 (cont'd)

Chemical Class	Compound	Sampling Locations							
		L-17	L-21	L-23	L-26	L-27	L-28	L-30	L-26A
	isopropanol	-	+	-	+	+	-	-	-
	t-butanol	-	+	-	-	-	-	-	+
	n-butanol	-	+	-	+	+	-	+	-
	methyl ethyl ketone	-	+	-	-	+	-	-	-
	2-tetradecanone	-	-	+	-	-	-	-	-
	furan (tent.)	-	-	-	+	-	-	-	-
	pentanol isomer (tent.)	-	-	-	+	-	-	-	-
	hexanone isomer	-	-	-	+	-	-	-	-
	cyclopentanone (tent.)	-	-	-	+	-	-	-	-
	acetic acid (tent.)	-	-	-	-	+	-	-	-
	n-undecanal	-	-	-	-	+	-	-	-
	di-isopropyl ether	-	-	-	-	-	+	-	+

---

[a] See Table 28 and Fig. 13 and 14 for protocol and sampling locations.

[b] - = not detected, + = detected.

area. Several ethers, alcohols, and other compounds were identified in the sample taken at Location No. 21.

Quantitative Analysis--

Table 23 presented the potential emissions from some chemical industries in this area. Much of the chemical industry was associated with the production of halogenated hydrocarbons and assorted fine chemical products. The availability of chemical emission data provided a good opportunity to apply the collection and analysis methods which were developed over the past few years. The ability to sample ambient air for which some compositional information was available allowed for further validation of the method.

In addition to the chemical industry, an incineration facility was located near Baton Rouge which destroys aliphatic hydrocarbons, aromatic hydrocarbons, alcohols, viscous oils, polyglycols, tars, chlorinated aliphatics, chlorinated benzenes and other aromatics, waxes and rubber. The waste materials which are treated at the Rollins Environmental facilities are of a diverse origin.

Twenty-two halogenated hydrocarbons were quantified at 11 locations in the Iberville Parish. In addition, the levels of benzene in ambient air were also estimated. These results are shown in Table 34. Of particular interest was the sample from Location No. 7 which contained the largest total number of halogenated hydrocarbons. 1,1,1-Trichloroethane exhibited the highest level (8,760 ng/m^3). Furthermore, the highest concentration for bis-(2-chloroisopropyl)ether (363 ng/m^3) was observed at location No. 7.

Table 35 lists the concentration of four halogenated organics that were detected on the carbon backup cartridge. The concentrations of chloroacetylene, vinyl chloride, chloroethane and vinylidene chloride appeared to be elevated also in the sample taken at location No. 7 (Fig. 10).

Several chemicals were quantified in the samples taken in the Baton Rouge, LA area and these results are summarized in Table 36. The predominant halogenated compound was chloroform which was found at considerably higher levels throughout all sampling periods at all locations relative to other halogenated compounds which were quantified. Table 37 presents the minimum halogenated hydrocarbon vapors which were quantified in the ambient air for

Table 34. CONCENTRATIONS OF AMBIENT AIR POLLUTANTS IN IBERVILLE PARISH, LA[a]

	Locations										
Compound	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11
1,1,1-trichloroethane	1100±20	1820±100	68±8	1500±20	430±50	2680±0	8760±1160	1556±0	524±61	416±27	112±56
1,2-dichloroethane	1726±345	1219±0	9±7	1590±45	399±28	3727±1127	4709±200	362±4	304±36	146±24	91±30
vinyl chloride	NQ[b]	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ
carbon tetrachloride	800±800	ND	20±10	ND	ND	T	4628±1100	335±250	667±200	277±18	ND
dichlorobutane	153±70	2714±2000	71±45	ND	ND	7285±1571	1392±178	ND	54±25	ND	ND
tetrachloroethylene	82±20	977±900	ND	21±0	54±3	489±70	1224±173	159±170	27±3	30±10	16±8
1,1,2,2-tetrachloroethane	52±1	264±191	ND	ND	T	ND	1573±243	ND	148±133	ND	ND
chloroform	1988±122	419±0	ND	633±10	956±112	2433±100	5866±688	1080±468	511±327	1387±161	1113±274
1,2-dichloropropane	944±172	735±37	1015±620	ND	209±4	1363±33	2239±136	T	ND	ND	ND
chloroethane	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ
vinylidene chloride	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ	NQ
1,1-dichloroethane	ND[c]	ND	ND	ND	ND	T	478±56	ND	ND	ND	ND
dichloropropene	ND	ND	ND	ND	ND	106±4	261±92	ND	ND	ND	ND
1,1,2-trichloroethane	580±60	ND	ND	ND	36±0	260±18	1840±440	ND	ND	ND	ND
tetrachlorobutadiene	ND	139±70	ND	ND	ND	T	17±11	ND	ND	ND	ND
hexachloro-1,3-butadiene	ND	ND	ND	ND	ND	18±3	37±15	ND	ND	ND	ND
1,3-dichloropropene	10±5	ND	ND	ND	T	ND	ND	ND	ND	ND	ND
trichloropropane	ND	ND	ND	ND	ND	T	24±9	ND	ND	ND	ND
tetrachloropropane isomer	ND	32±30	ND	ND	ND	242±36	13±6	ND	ND	ND	ND
pentachloroethane	ND	ND	ND	ND	T	ND	13±5	ND	ND	ND	ND
bis- (2-chloroisopropyl) ether	66±22	ND	ND	ND	ND	T	363±152	ND	ND	ND	ND
hexachloroethane	ND	ND	ND	ND	ND	T	T	ND	ND	ND	ND
pentachlorobutadiene	ND	ND	ND	ND	ND	ND	T	ND	ND	ND	ND
chlorotoluene	ND	ND	ND	ND	ND	ND	ND	35±7	ND	ND	ND
chlorobenzene	ND	ND	ND	ND	ND	ND	ND	29±10	ND	ND	ND
benzene	1808±163	1727	1990±436	586±23	1423±41	1904±86	1904±86	16077±3714	6181±2480	1668±188	421±71

[a] Values are in ng/m^3 with reproducibility for duplicate cartridges.

[b] NQ = not quantitated, these compounds were collected and analyzed from carbon cartridges.

[c] ND = not detected.

Table 35. CONCENTRATIONS OF AMBIENT AIR POLLUTANTS IN IBERVILLE PARISH, LA[a]

Compound	Location											
	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	B[b]
Chloroacetylene	ND	ND	12	ND	58	ND	45	T	T	ND	ND	ND
Vinyl chloride	192	1,230	30	T	59	534	1,334	64	76	ND	ND	ND
Chloroethane	ND	ND	ND	ND	ND	ND	1,378	ND	ND	ND	ND	ND
Vinylidene chloride	128	36	ND	ND	ND	132	990	ND	ND	ND	ND	ND

[a] Pollutants which passed through the Tenax GC cartridge were collected on carbon then transferred to Tenax in the lab via thermal desorption, values are in ng/m^3.

[b] B = blank carbon cartridge.

Table 36. VOLATILE ORGANIC VAPORS ESTIMATED IN AMBIENT AIR OF BATON ROUGE, LA AND VICINITY

Chemical	Locations																	
	L17	L18	L19	L20A	L21	L22	L20B	L23	L24	L25A	L26A	L27	L28	L25B	L26B	L29	LF[a]	L30
1,1,1-trichloroethane	178	ND	ND	ND	178	ND	ND	200	178	222	ND	78 ± 24	ND	ND	ND	200	ND	167
1,2-dichloroethane	137	712	458	585	78	ND	887	731	712	10,341	751	322 ± 0	3,229	2,000	1,522	ND	5,024	302
carbon tetrachloride	874	452	289	ND	74	ND	311	592	533	311	533	148 ± 0	429	163	119	74	1,037	192
tetrachloroethylene	84	34	32	ND	60	11	44	53	43	33	64	20 ± 0	364	13	47	17	250	18
chloroform	6,710	6,968	1,290	181	4,775	387	542	1,484	1,097	560	368	568 ± 13	839	387	464	258	2,129	477
dichlorobutane	193	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	13	ND	ND	ND	ND
1,2-dichloropropane	ND	ND	ND	ND	ND	ND	ND	30	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
chloroethane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
vinylidene chloride	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
1,1-dichloroethane	ND	ND	ND	ND	ND	ND	68	ND	ND	90	ND	ND	ND	34	64	ND	233	ND
1,1,2-trichloroethane	ND	ND	ND	ND	ND	ND	ND	ND	80	ND	54	ND	ND	ND	ND	ND	533	ND
hexachloro-1,3-butadiene	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	23	ND	117	ND
chloroprene	ND	ND	ND	ND	x	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
benzene	11,050	2,678	2,535	80	1,220	8,099	9,217	2,132	1,456	676	650	533	2,665	1,248	3,796	273	1,040	1,326
acetone	1,035	1,482	176	729	682	1,521	1,835	2,941	3,294	1,447	988	68 ± 23	729	188	423	329	1,765	329
methylene chloride	2,800	2,160	280	ND	1,999	160	280	840	440	240	160	320 ± 76	200	280	320	160	680	160
β-chlorostyrene	ND	ND	ND	ND	x	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
dichlorobenzene isomer(s)	ND	ND	ND	ND	ND	ND	ND	x	ND	ND	ND	ND	ND	ND	ND	ND	ND	x
chloroprene dimer	ND	ND	ND	ND	x	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
chlorobenzene	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	10	ND	ND
1,1,2,2-tetrachloroethane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	T	ND	ND	ND	ND	ND	ND	71

[a] Downwind of several petroleum facilities.

Table 37. MINIMUM TOTAL HALOGENATED HYDROCARBON VAPOR IN AMBIENT AIR OF BATON ROUGE, LA

Location[a]	ng/m^3	Location	ng/m^3
L17	10,976	L25A	11,797
L18	10,326	L26A	1,925
L19	2,349	L27	1,456
L20A	762	L28	6,517
L21	7,164	L25B	9,407
L22	558	L26B	2,559
L20B	2,132	L29	709
L23	3,930	LE	10,003
L24	3,083	L30	1,387

[a] See Table 28 and Fig. 13 and 14 for protocol and sampling locations.

this area. In some cases the concentrations of halogenated compounds surpassed 10,000 ng/m^3.

Linden and Deepwater, NJ Areas

Qualitative Analysis--

A few samples were selected for full characterization and these detailed results are given in Appendix B. A summary of the volatile organics which were identified in ambient air taken on American Cyanamid Co. property in Linden, NJ is given in Table 38. As in previous sampling of other sites, many halogenated hydrocarbons were identified; however, it was difficult to ascertain which of these were site-specific. Several sulfur compounds were also characterized. Many of these compounds represent the first report of their detection in ambient air using the method of sampling and analysis described from this laboratory. Two nitrogen compounds, acrylonitrile and cyanobenzene, were also identified. Furthermore, many oxygenated compounds were characterized with the predominant number represented by samples P1/2 P2/3 and P3/4. These sampling locations (Fig. 14) were downwind positions.

A summary of the vapor phase organics which were identified in the atmosphere taken onsite at E. I. DuPont deNemours are given in Table 39. Again many halogenated hydrocarbons were identified and several were of particular interest since these were potential emission (Table 24). These were vinylidene chloride (dichloroethylene isomer), 1,2-dibromoethane (ethylene dibromide), trichloroethylene, carbon tetrachloride and tetrachloroethylene. Two sulfur compounds were identified (2,3-benzothiophene and methylbenzyl thiophene isomer). Several oxygenated compounds were also characterized. Methyl methacrylate and acetone were also listed as potential priority compounds of interest (Table 24). The most surprising results were reflected by the number of nitrogen compounds in these samples since in Table 39 only two compounds were reported, nitrobenzene and acrylonitrile. The sample with the most number of chemical classes was P4/L4.

In addition to the analysis of these samples on an OV-101 SCOT column, a number of duplicate samples were chromatographed on a Carbowax 20M capillary. The results of these analyses are also given in Appendix B. One constituent of interest whose abundance was relatively large could not be identified. Its mass spectrum is given in Figure 18. The isotopic cluster

Table 38. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR AT AMERICAN CYANAMID CO, LINDEN, NJ

	Period/Locations[a]					
Chemical Class	P1/L1	P1/L2	P1/L4	P2/1L	P2/L3	P3/L4
Halogenated Compounds						
chloromethane	-[b]	+	-	-	+	+
bromomethane	-	+	-	-	+	-
chloroethane	-	-	-	-	+	+
dichloromethane	+	+	-	+	+	+
chloroform	+	+	+	+	-	+
1,2-dichloroethane	-	-	-	-	+	-
1,1,1-trichloroethane	+	+	+	+	+	+
carbon tetrachloride	+	+	+	+	+	+
trichloroethylene	-	+	+	+	+	+
tetrachloroethylene	+	+	+	+	+	+
chlorobenzene	+	+	+	-	+	+
dichlorobenzene isomer	+	+	-	+	+	+
o-dichlorobenzene	+	+	-	+	+	+
trichlorobenzene isomer	-	-	-	-	+	+
Sulfur Compounds						
2-thiapropane	-	+	-	-	-	-
2,3-dithiabutane	-	+	+	-	+	+
carbon disulfide	-	-	-	-	+	+
dithiapentane isomer	-	-	-	-	+	+
3,4-dithiahexane	-	-	-	-	+	+
Oxygenated Compounds						
acetaldehyde	+	+	+	+	+	+
furan	+	-	+	+	+	+
propanal	+	+	+	+	+	+
acetone	+	+	+	+	+	+
t-butanol	+	+	+	+	+	+
2-butenal (tent.)	+	-	+	+	+	+
dimethyl ether	-	-	+	-	-	-
isopropanol	-	-	+	+	+	-
butanal	-	-	+	-	+	+
acrolein	-	+	-	-	-	-
methyl ethyl ketone	+	+	+	+	+	+
n-hexanal	-	-	-	-	-	+
n-heptanal	-	-	-	-	-	+

(continued)

Table 38 (cont'd)

Chemical Class	Period/Locations[a] P1/L1	P1/L2	P1/L4	P2/L1	P2/L3	P3/L4
Oxygenated Compounds (cont'd)						
$C_6H_{12}O$ (ketone) isomer	+	+	–	–	–	+
benzaldehyde	+	+	+	+	+	+
phenol	+	+	–	–	+	–
acetophenone	+	+	+	+	+	+
n-nonanal	+	+	+	+	+	+
C_2-alkyl phenol isomer	+	+	–	–	+	+
n-decanal	+	+	+	+	+	+
2-methylpropenal	–	+	–	–	–	–
methyl vinyl ketone	–	+	+	–	–	–
cyclohexanone	–	+	–	–	+	–
anisole	–	+	–	–	–	–
n-octanal	–	+	+	+	+	–
dimethyl phenol isomer	–	+	–	–	+	+
diethyl maleate	–	+	+	–	+	+
diethyl fumarate	–	–	+	–	–	+
acetic acid (tent.)	+	–	+	+	+	+
dibenzofuran	–	+	–	–	–	–
benzophenone	–	+	–	–	–	+
$C_{15}H_{30}O$ isomer	+	+	–	–	–	+
1-acetoxy-butene-1 (tent.)	–	–	–	+	–	+
diethyl phthalate	–	+	–	+	–	+
4-methyl-2-pentanone	–	–	–	+	+	+
tolualdehyde isomer (tent.)	–	–	–	–	+	–
ethyl phenol isomer	–	–	–	–	+	–
C_3-alkyl phenol isomer	–	–	–	–	+	–
C_2-alkyl phenol isomer	–	–	–	–	+	–
n-undecanal	–	–	–	–	+	+
Nitrogenous Compounds						
acrylonitrile	–	–	+	–	–	–
cyanobenzene	–	–	–	+	+	+

[a] See Table 30 and Fig. 15 and 16 for protocol and sampling locations.

[b] – = not detected, + = detected.

Table 39. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR AT E. I. DUPONT DE NEMOURS, DEEPWATER, NJ

Chemical Class	Period/Locations[a]				
	P4/L4	P5/L1	P5/L4	P6/L1	P6/L2
Halogenated Compounds					
chloromethane	+[b]	-	-	-	-
dichloromethane	+	+	+	+	+
chloroform	+	+	+	+	+
1,2-dichloroethane	+	+	+	-	-
1,1,1-trichloroethane	+	+	+	+	+
carbon tetrachloride	+	+	+	+	+
trichloroethylene	+	+	-	+	-
1,2-dibromoethane	+	-	+	-	-
tetrachloroethylene	+	+	+	+	+
chlorobenzene	+	+	+	+	+
dichlorobenzene isomer	+	+	+	+	+
o-dichlorobenzene isomer	+	+	+	+	+
$C_7H_6Cl_2$ (dichlorotoluene or benzyl chloride	+	-	+	-	-
trichlorobenzene isomer	+	-	+	+	-
trichlorobenzene isomer	+	-	+	+	-
dichloroethylene isomer	-	-	-	-	+
Sulfur Compounds					
2,3-benzothiophene	-	-	-	-	+
methylbenzothiphene isomer	-	-	-	-	+
Oxygenated Compounds					
acetaldehyde	+	+	+	+	+
furan	+	-	-	+	+
propenal	+	+	-	+	+
propanal	+	+	+	+	+
acetone	+	+	+	+	+
C_4H_8O (aldehyde) isomer	+	+	-	-	-
2-methylpropenal	+	+	+	+	+
methyl ethyl ketone	+	+	+	-	-
methyl vinyl ketone	+	+	-	-	-
methyl methacrylate	+	-	-	-	-
acetic acid (tent.)	+	+	+	-	+

(continued)

Table 39 (cont'd)

Chemical Class	Period/Locations[a]				
	P4/L4	P5/L1	P5/L4	P6/L1	P6/L2
Oxygenated Compounds (cont'd)					
4-methyl-2-pentanone	+	+	+	-	-
n-hexanal	+	+	+	+	-
dibenzofuran	-	-	-	-	+
2-methylcyclohexanone	+	-	-	-	-
benzaldehyde	+	+	+	+	+
phenol	+	-	+	+	+
n-octanal	+	+	+	+	+
benzoic acid (tent.)	+	-	-	-	-
n-decanal	+	+	+	+	+
n-butanal	-	+	+	+	+
n-pentanal	-	+	+	+	-
n-heptanal	-	+	-	+	+
phenyl acetaldehyde	-	+	-	+	+
ethyl phenol isomer	-	+	-	+	+
dimethylphenol isomer	-	+	+	+	+
dimethylphenol isomer	-	+	+	+	-
C_3-alkyl phenol isomer	-	-	+	+	-
diethyl ether	-	+	-	-	-
Nitrogen Compounds					
cyanobenzene	+	+	+	+	+
aniline or methylpyridine	+	-	-	-	-
nitrobenzene	+	-	+	-	-
chloroaniline isomer	+	-	-	-	+
nitrophenol isomer	+	-	-	-	-
$C_9H_{13}N$ isomer (tent.)	+	-	-	-	-
o-nitrotoluene	+	-	-	+	-
p-nitrotoluene	+	-	-	-	-
chloronitrobenzene isomer	+	-	+	-	-
chloronitrobenzene isomer	+	-	+	-	-
dichloronitrobenzene or dichloroaniline isomer	+	-	+	-	-
dichloronitrobenzene or dichloroaniline isomer	+	-	-	-	-
quinoline	-	-	-	-	+
methylquinoline	-	-	-	-	+

---

[a] See Table 30 and Fig. 17 and 18 for protocol and sampling locations.

[b] - = not detected, + = detected.

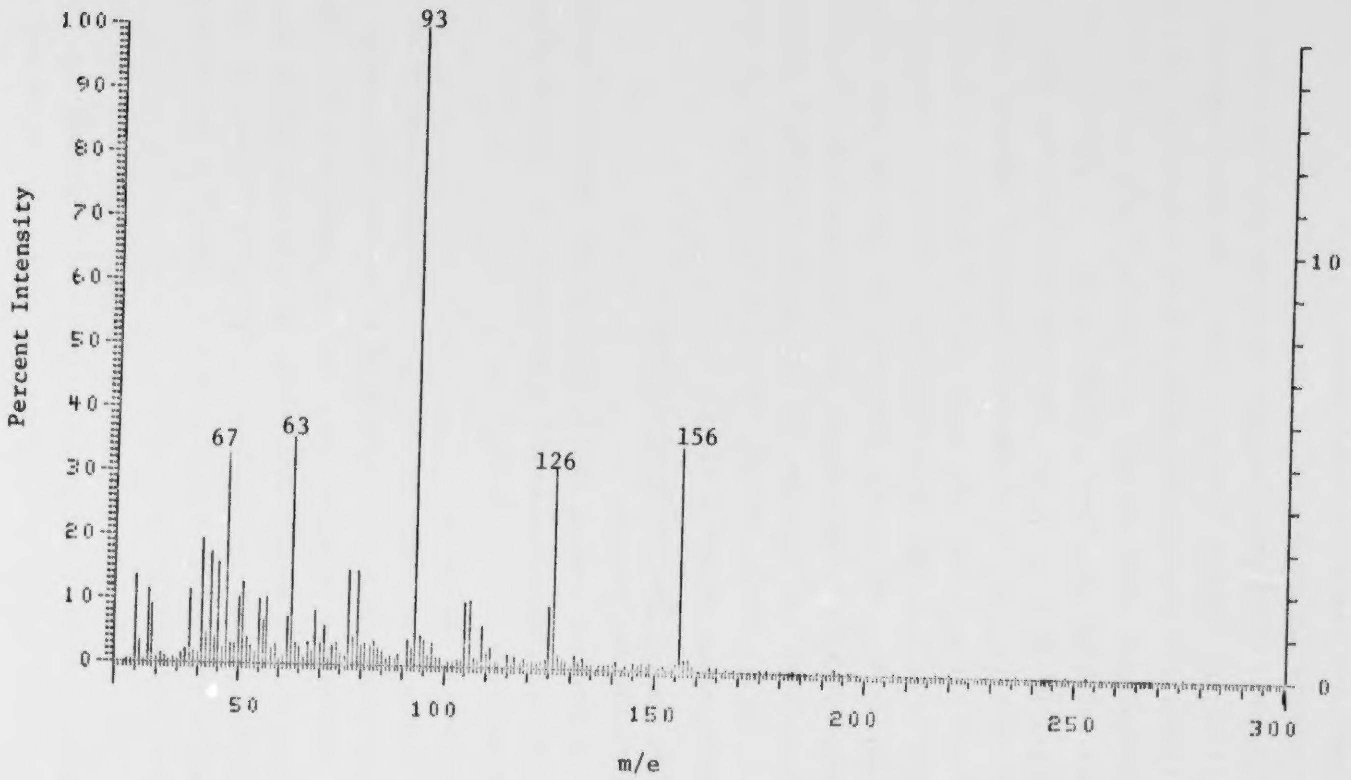


Figure 18. Mass spectrum of unknown (peak No. 46, Table B33) compound in ambient air from Linden, NJ.

for the parent ion suggests the presence of sulfur. As represented by one of the samples which was chromatographed on a Carbowax 20M capillary, this component was the major constituent.

Quantitative Analysis--

Several vapor phase organic compounds were selected for quantification in all of the samples collected from Linden and Deepwater, NJ. The ambient air levels for selected halogenated hydrocarbons, sulfur, oxygen and nitrogen-containing compounds and aromatics are given in Tables 40 and 41 for Linden and Deepwater sites, respectively. In general ng/m^3 quantities were detected for most organics. The general conclusion that can be drawn from these data is that the halogenated compounds measured appeared to be ubiquitous and not site-specific since they occurred at relatively equivalent levels in both upwind and downwind positions with respect to the American Cyanamid site. The sulfur compounds and benzene were detected primarily in downwind locations and suggest that they may be site-specific in origin. This was also the case for the nitrogenous chemicals measured at the Deepwater site. No appreciable levels of any of these materials were found in the control sample (Tenax GC blank).

Camden, NJ and Philadelphia, PA Areas

Qualitative Analysis--

A detailed listing of the vapor phase organic pollutants occurring in ambient air samples collected from Camden, NJ-Philadelphia, PA area is given in Appendix B.

Quantitative Analysis--

Table 42 presents the estimated concentrations of several halogenated hydrocarbons which were quantified in ambient air samples from this area. The predominant compounds detected were methylene chloride, chloroform, 1,2-dichloroethane, methyl chloroform, tetrachloroethylene and chlorobenzene. These halogenated hydrocarbons are probably ubiquitous since they have been found in many previous samples taken from other geographical areas.

GENERAL CONCLUSIONS

The results of the sampling analysis conducted for the three described geographical areas has yielded considerable information concerning the presence of vapor phase organic pollutants in the ambient atmosphere.

Table 40. AMBIENT AIR LEVELS OF SEVERAL VOLATILE ORGANIC VAPORS SURROUNDING AMERICAN CYANAMID CORP., LINDEN, NJ

Chemical Class	Compound	P1/L1	P1/L2	P1/L3	P1/L4	P2/L1	P2/L2	P2/L3	P2/L4	P3/L1	P3/L2	P3/L3	P3/L4
Halogenated Hydrocarbon	methylene chloride	100	258	168	58	52	324	369	134	81	261	972	418
	chloroform	50	154	133	99	41	195	178	150	86	229	773	190
	1,2-dichloroethane	-	14	9	42	12	9	47	34	T	38	9	8
	1,1,1-trichloroethane	13	735	9	13	9	13	39	244	T	3,116	1,440	24
	carbon tetrachloride	21	22	28	10	14	14	71	51	T	32	T	T
	trichloroethylene	-	139	11	6	8	2	242	25	-	17	T	T
	chlorobenzene	3	15	123	272	11	4	30	222	-	T	T	T
	o-dichlorobenzene	2	-	-	-	-	-	-	74	-	20	-	T
	dichlorobenzene isomer	T	30	-	1	-	-	13	T	-	T	T	T
	trichlorobenzene isomer	-	2	-	-	-	-	7	T	-	T	-	T
Sulfur Compounds	2-thiopropane	-	T	T	-	-	-	-	-	-	-	-	-
	2,3-dithiabutane	-	T	-	T	-	T	T	-	-	-	-	T
	dithiapentane isomer	-	-	-	-	-	-	T	-	-	-	-	T
	3,4-dithiahexane	-	-	-	-	-	-	T	-	-	-	-	T
Aromatics	benzene	490	890	1,342	613	174	43	21,309	8,239	224	223	1,226	1,342
	cyanobenzene	-	23	49	8	14	-	18	T	T	T	T	T
Oxygenated Compounds	furan	20	18	46	9	23	-	-	-	-	-	-	-
	t-butanol	1,745	160	129	87	202	-	247	219	-	-	-	-
	isopropanol	-	25	4	4	59	-	-	-	-	-	-	-
	methyl ethyl ketone	30	45	69	40	84	-	T	T	T	-	-	T
	benzaldehyde	119	127	164	36	83	-	557	344	-	136	328	158
	acetophenone	173	232	251	131	205	-	1,167	459	-	322	300	241
	methyl vinyl ketone	15	19	10	45	-	-	16	-	-	-	-	-
	cyclohexanone	158	-	-	22	-	-	629	-	-	-	-	T
	anisole	-	-	4.4	-	-	-	T	T	-	-	-	T
	diethyl maleate	-	-	-	-	-	-	-	1,085	83	60	T	447
	diethyl fumarate	-	488	882	863	40	-	251	586	T	62	T	406
	tolualdehyde	87	31	54	17	61	-	83	T	T	T	T	T

Table 41. AMBIENT AIR LEVELS OF SEVERAL VOLATILE ORGANIC VAPORS SURROUNDING E. I. DuPONT deNEMOURS, DEEPWATER, NJ[a]

Chemical Class	Compound	P4/L5	P4/L6	P4/L7	P4/L8	P5/L5	P5/L6	P5/L7	P5/L8	P6/L5	P6/L6	P6/L7	P6/L8	Tenax Blank
Halogenated Hydrocarbons	methylene chloride	65	405	35	437	75	486	-	625	345	248	261	81	T
	chloroform	152	-	-	T	150	439	-	64	-	70	90	13	T
	1,2-dichloroethane	12	-	-	T	-	-	-	53	-	-	-	24	-
	1,1,1-trichloroethane	-	-	2,842	T	-	-	-	67	-	-	-	14	-
	carbon tetrachloride	19	-	-	-	-	-	-	-	-	-	-	32	-
	trichloroethylene	4	-	-	-	-	-	-	56	-	-	-	5	-
	1,2-dibromoethane	-	-	T	-	-	-	-	-	-	-	-	-	-
	tetrachloroethylene	6	13	T	60	69	-	-	218	22	29	-	57	-
	chlorobenzene	14	15	11	512	55	-	-	305	25	17	12	669	-
	o-dichlorobenzene	17	554	-	51	25	-	-	-	T	-	-	1,319	-
	dichlorobenzene isomer	19	12	-	1,240	21	-	-	T	101	404	-	14	-
	trichlorobenzene isomer	T	T	-	136	-	-	-	150	13	-	-	113	-
	dichloroethylene	-	-	-	-	-	-	-	-	-	-	-	-	-
	dichlorotoluene	-	-	-	59	-	-	-	61	-	107	-	29	-
Sulfur	2,3-benzothiophene	-	-	-	T	-	-	-	-	-	536	-	T	-
	methylbenzothiophene	-	-	-	-	-	-	-	-	-	116	-	T	-
Oxygenated Compounds	furan	T	-	-	-	-	-	-	-	59	-	-	-	-
	acetone	T	-	-	-	-	-	-	-	-	-	-	-	-
	methyl ethyl ketone	T	-	-	-	-	-	-	-	-	-	-	-	-
	methyl vinyl ketone	T	-	-	-	-	-	-	-	72	-	-	-	-
	methyl methacrylate	-	-	-	25	-	-	95	27	-	21	-	16	-
	dibenzofuran	-	184	-	-	-	138	-	29	-	3,279	-	-	-
	phenylacetladehyde	-	28	33	-	-	-	-	-	-	41	T	-	-
Nitrogen Compounds	cyanobenzene	T	-	12	21	35	-	-	-	-	-	-	-	-
	aniline (or methylpyridine)	-	-	-	28	-	-	-	-	-	-	-	-	-
	nitrobenzene	-	-	-	123	-	-	-	-	-	-	-	105	-
	chloroaniline isomer	-	-	-	146	-	-	-	-	-	5,960	-	T	-
	nitrophenol	-	-	-	73	-	-	-	-	-	-	-	24	-
	o-nitrotoluene	-	-	-	T	-	-	-	-	-	47	-	-	-
	p-nitrotoluene	-	-	-	59	-	-	-	86	-	-	-	-	-

(continued)

Table 41 (cont'd)

Chemical Class	Compound	P4/L5	P4/L6	P4/L7	P4/L8	P5/L5	P5/L6	P5/L7	P5/L8	P6/L5	P6/L6	P6/L7	P6/L8	Tenax Blank
	chloronitrobenzene isomer (or chloroaniline)	–	–	–	360	–	–	–	T	–	–	–	–	–
	dichloronitrobenzene (or dichloroaniline)	–	–	–	2,704	–	–	–	T	–	–	–	32	–
	quinoline	–	41	–	–	–	–	–	–	–	–	–	–	–
	methylquinoline	–	–	–	–	–	–	–	–	–	1,478	–	–	–

[a] Values are in ng/m^3.

Table 42. ESTIMATION OF LEVELS OF HALOGENATED HYDROCARBONS IN THE GENERAL AREA OF CAMDEN, NJ/PHILADELPHIA, PA

Compound	PERIOD/LOCATION[a]											
	P1/L1A	P1/L1B	P2/L2A	P3/L3A	P3/L3B	P4/L4A	P4/L4B	P5/L5A	P6/L6A	P7/L7A	P8/L8A	Blank[b]
methylene chloride	T(714)	T(571)	T(1000)	562 ± 7	T(555)	T(555)	T(555)	T(555)	966 ± 78	T(555)	914 ± 460	3.5
chloroform	146 ± 21	262 ± 137	T(167)	T(97)	T(97)	T(96)	T(96)	T(97)	235 ± 22	154 ± 58	277 ± 166	1.6
carbon tetrachloride	T(95)	T(95)	T(125)	T(74)	T(74)	T(74)	T(74)	T(74)	T(74)	T(74)	T(83)	<2
vinylidene chloride	<333	T(333)	<454	<263	<263	<263	T(263)	<263	T(263)	<263	T(303)	<10
1,2-dichloroethylene	<333	<333	<454	<263	<263	<263	<263	<263	<263	<263	<303	<10
1,1-dichloroethane	<357	<357	<348	228	<228	<228	<228	<228	<228	<228	<345	<8
1,2-dichloroethane	T(258)	T(258)	<667	167 ± 77	T(195)	465 ± 21	927	T(195)	T(195)	T(195)	T(222)	<8
1,1,1-trichloroethane	T(333)	T(267)	T(294)	325 ± 108	T(278)	T(277)	T(278)	NQ	1639 ± 1250	129 ± 2	656 ± 344	<5
1,1,2-trichloroethane	<250	<250	<131	<167	<217	<217	<217	<217	<217	<278	<312	<5
trichloroethylene	T(100)	T(100)	T(92)	T(111)	T(92)	T(83)	<92	T(80)	T(88)	T(77)	T(312)	<5
tetrachloroethylene	118 + 2	775 ± 665	185 ± 56	94 ± 31	T(74)	142 ± 25	292	T(122)	T(127)	276 ± 169	T(189)	<7
1,1,1,2-tetrachloroethane	<109	<103	<111	<95	<111	<100	<111	<96	<109	<92	<162	<6
1,1,2,2-tetrachloroethane	<109	<103	<111	<95	<111	<100	<111	<96	<109	<92	<162	<6
pentachloroethane	<90	<86	<92	<79	<92	<83	<92	<80	<90	<77	<135	<5
hexachloroethane	<90	<86	<92	<79	92	<83	<92	<80	<90	<77	<135	<5
chlorobenzene	<272	448 ± 190	T(278)	T(238)	T(278)	T(250)	T(278)	T(242)	<272	T(231)	T(405)	<15
o-dichlorobenzene	<182	T(172)	T(185)	<159	185	T(167)	T(185)	<161	<182	<154	<286	<10
m-dichlorobenzene	T(182)	T(172)	T(185)	T(159)	T(185)	T(167)	T(185)	T(161)	T(182)	T(154)	T(286)	<10
p-dichlorobenzene	<163	<155	<167	<143	167	<150	<167	<145	<164	<138	<257	<9
1,2,4-trichlorobenzene	<109	T(103)	<111	<95	111	<100	<111	<96	<109	<96	<162	<6
1,3,5-trichlorobenzene	<90	T(86)	<92	<79	92	<83	T(92)	<80	<90	<77	<135	<5
1,2,3-trichlorobenzene	<109	<103	<111	<95	111	<100	<111	<96	<109	<96	<162	<6

[a] Values in ng/m^3, see Table 31 and Fig. 19 for protocol and sampling locations.

[b] Values in ng/cartridge.

Coupled with the information concerning the chemical industries usage, storage, or production of chemicals, the Tenax GC sampling and the hrgc/ms/comp analysis methodology has been applied and demonstrated to coborate much of the chemical activity occurring at these industrial sites. Furthermore, many new compounds have been identified particularly those which are sulfur- and nitrogen-containing as well as many site-specific halogenated hydrocarbons which have not been previously reported. Since the developed methodology for collection and analysis of vapor phased organics has yielded information concerning the specific chemicals occurring, the next phase of research should pursue a more rigorous establishment of the accuracy and reproducibility of this technique for the chemical classes reported.

As more information is accumulated concerning the composition of the atmosphere, it is becoming increasingly evident that many organic vapors may be considered ubiquitous eventhough they may be of anthropogenic nature while others are more site-specific and more directly associated with industrial activity at specific sites within the Continental U.S.

REFERENCES

1. Pellizzari, E. D., Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres", EPA-650/2-74-121, Contract No. 68-02-1228, 148 pp., July, 1974.
2. Pellizzari, E. D., Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors, EPA-600/2-75-076, Contract No. 68-02-1228, 186 pp., November, 1975.
3. Pellizzari, E. D., The Measurement of Carcinogenic Vapors in Ambient Atmospheres", EPA-600/7-77-055, Contract No. 68-02-1228, 288 pp., June, 1977.
4. Pellizzari, E. D., Measurement of Carcinogenic Vapors in Ambient Atmospheres, EPA-600/7-78-062, Contract No. 68-02-1228, 224 pp., April, 1978.
5. Pellizzari, E. D., Analysis of Organic Air Pollutants by Gas Chromatography and Mass Spectroscopy", EPA-600/2-77-100, Contract No. 68-02-2262, 104 pp., June, 1977.
6. Pellizzari, E. D., Bunch, J. E., Carpenter, B. H., Sawicki, E., Environ. Sci. Tech., 9, 552 (1975).
7. Pellizzari, E. D., Carpenter, B. H., Bunch, J. E., Sawicki, E., Environ. Sci. Tech., 9, 556 (1975).
8. Pellizzari, E. D., Bunch, J. E., Berkley, R. E., McRae, J., Anal. Lett., 9, 45 (1976).
9. Pellizzari, E. D., Bunch, J. E., Berkley, R. E., McRae, J., Anal. Chem., 48, 803 (1976).
10. Pellizzari, E. D., Bunch, J. E., Berkley, R. E., Bursey, J. T., Biomed. Mass Spec., 3, 196 (1976).
11. Pellizzari, E. D., Bunch, J. E., Bursey, J. T., Berkley, R. E., Sawicki, E., Krost, K., Anal. Lett., 9, 579 (1976).
12. Fine, D. H., Runbehler, D. P., Pellizzari, E. D., Bunch, J. E., Berkley, R. E., McRae, J., Bursey, J. T., Bull. Environ. Contam. and Tox. 15, 739 (1976).

13. Bursey, J. T., Smith, D., Bunch, J. E., Williams, R. N., Berkley, R. E., Pellizzari, E. D., American Lab., Feb., 1978.

14. Berkley, R. E., Pellizzari, E. D., Anal. Letters, 4, 327 (1978).

15. Berkley, R. E., Pellizzari, E. D., McRae, J., Bunch, J., 1976 Pitt Conf. Anal. Chem. Appl. Spect., 2/29-3/5/76, Cleveland, OH.

16. Pellizzari, E. D., Bunch, J. E., Berkley, R. E., Bursey, T., 24th Ann. ASMS Conf., May, 1976, San Diego, CA.

17. Pellizzari, E. D., Bunch, J. E., Berkley, R. E., Bursey, J. T., 24th Ann. ASMS Conf., May, 1976, San Diego, CA.

18. Berkley, R. E., Pellizzari, E. D., Bunch, J. E., Williams, R. N., 173rd Nat. ACS Mrg., March, 1977, New Orleans, LA.

19. Berkley, R. E., Pellizzari, E. D., Bursey, J. T., 173rd Nat. ACS Mtg., March, 1977, New Orelans, LA.

20. Pellizzari, E. D., Berkley, R. E., Bunch, J., Bursey, J. T., Smith, D., Williams, R., Willis, S., 25th Ann. ASMS Conf., May, 1977, Washington, DC.

21. Pellizzari, E. D., Williams, R., Bunch, J., Pardow, N., Bursey, J., FACSS, Nov., 1977, Detroit, MI.

22. Bursey, J., Erickson, M. D., Michael, L., Zweidinger, R., Pellizzari, E., AIChet Nat. Mtg., June, 1978, Philadelphia, PA.

23. Pellizzari, E., Symp. on App. Short-Term Bioassays to Complex Environ. Mix., Williamsburg, VA, Feb., 1978.

24. Smith, D. J., Pellizzari, E. D., Bursey, J. T., ASMS, St. Louis, MO, May, 1978.

25. Pellizzari, E. D., 10th Ohio Valley Chrom. Symp., Hueston Woods St. Prk. Ldge., OH, June, 1978.

26. Pellizzari, E. D., Symp. on Sampling and Preconcentration Tech. for Ultra-Trace Gases, U.S.E.P.A., RTP, NC, October 19, 1978.

27. Pellizzari, E. D., Improvement of Methodologies for the Collection and Analysis of Carcinogenic Vapors, EPA Contract No. 68-02-2764, in prep.

28. Atlas of Cancer Mortality for U. S. Counties: 1950-1969, DHEW, (NIH) 75-780.

29. U. S. Cancer Mortality by County: 1959-1969, DHEW (NIH) 74-615.

30. Louisiana Directory of Manufacturers, Louisiana Department of Commerce, Baton Rouge, 1968.

31. VonBodungen, G., Louisiana State Air Board, private communication, 1977.

32. 1974 New Jersey State Industrial Directory, New Jersey State Industrial Directory, 2 Penn Plaza, New York, NY 10001.

APPENDIX A

METHOD FOR SAMPLING AND ANALYSIS OF VOLATILE ORGANIC COMPOUNDS IN AMBIENT AIR BY GC/MS/COMP

SAMPLING AND ANALYSIS OF VOLATILE ORGANIC COMPOUNDS IN AMBIENT AIR

1.0 Principle of Method

Volatile organic compounds are concentrated from ambient air on Tenax GC in a short glass tube (1-3). Recovery of the volatile organics is accomplished by thermal desorption and purging with helium into a liquid nitrogen cooled nickel capillary trap (1,2,4) and then the vapors are introduced into a high resolution glass gas chromatographic column where the constituents are separated from each other (2,5). Characterization and quantification of the constituents in the sample are accomplished by mass spectrometry either by measuring the intensity of the total ion current signal or mass fragmentography (2,6). The collection and analysis systems are shown in Figure A-1.

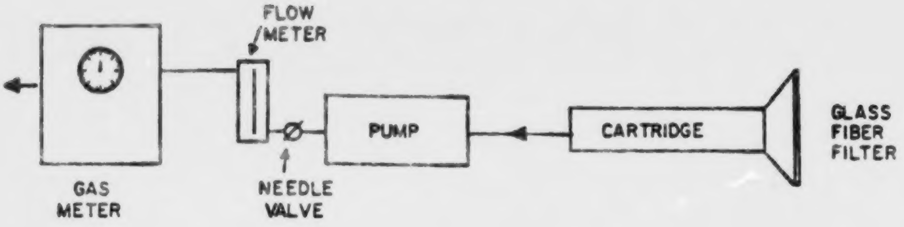
2.0 Range and Sensitivity

The linear range for the analysis of volatile organic compounds depends upon two principal features. The first is a function of the breakthrough volume of each specific compound which is trapped on the Tenax GC sampling cartridge and the second is related to the inherent sensitivity of the mass spectrometer for each organic (2,7). Thus, the range and sensitivity is a direct function of each compound which is present in the original ambient air. The linear range for the quantitation on the gas chromatograph/mass spectrometer/computer (gc/ms/comp) is generally three orders of magnitude. Table A1 lists the overall theoretical sensitivity for some examples of volatile organics which is based on these two principles (7).

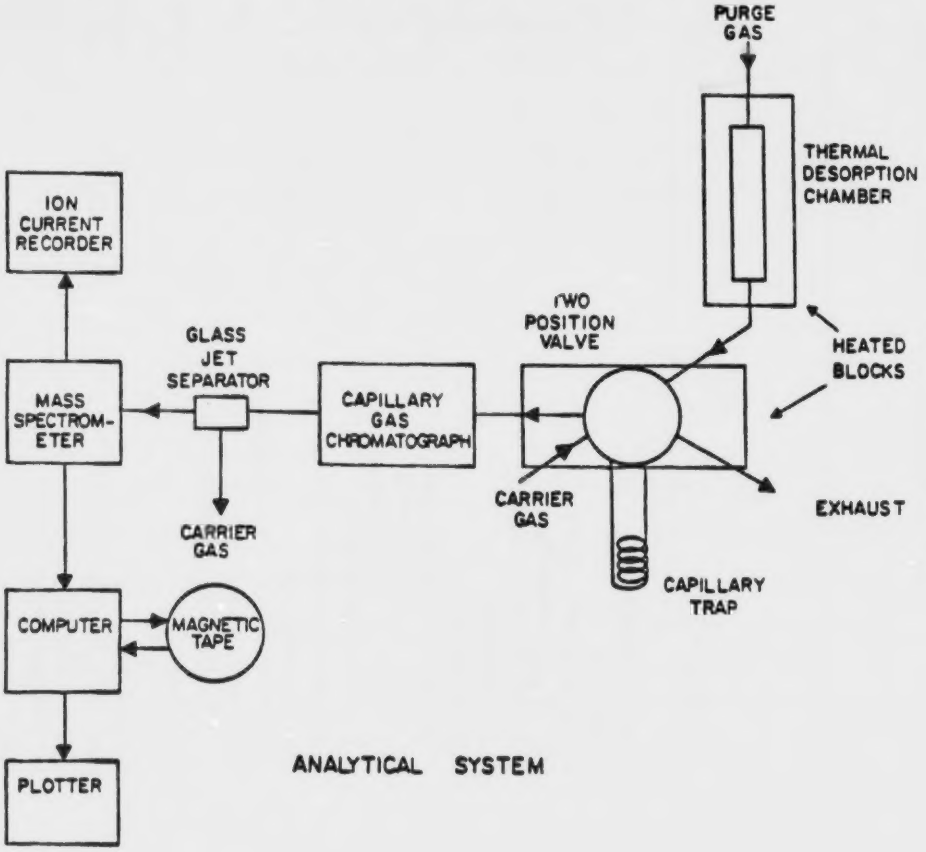
The sensitivity of this technique for the very volatile organic compounds (C_1 to C_5 alkanes) is inadequate for the purpose of this study. Alternate methods for their collection and analysis are suggested (11).

3.0 Interferences

The potential difficulties with this technique are primarily associated with those cases where isomeric forms of a particular substance cannot be resolved by the high resolution chromatographic column and when the mass cracking pattern of each of the isomers are identical. An example of such a problem is seen with the C_5-alkyl aromatics of which


FLOW METER
GAS METER
NEEDLE VALVE
PUMP
CARTRIDGE
GLASS FIBER FILTER

VAPOR COLLECTION SYSTEM


PURGE GAS
THERMAL DESORPTION CHAMBER
ION CURRENT RECORDER
TWO POSITION VALVE
HEATED BLOCKS
GLASS JET SEPARATOR
MASS SPECTROMETER
CAPILLARY GAS CHROMATOGRAPH
CARRIER GAS
EXHAUST
CARRIER GAS
CAPILLARY TRAP
COMPUTER
MAGNETIC TAPE
PLOTTER

ANALYTICAL SYSTEM

Figure A1. Vapor collection and analytical systems for analysis of organic vapors in ambient air.

Table A1. OVERALL THEORETICAL SENSITIVITY OF HIGH RESOLUTION GAS CHROMATOGRAPHY/MASS SPECTROMETRY/COMPUTER ANALYSIS FOR ATMOSPHERIC POLLUTANTS

Chemical Class	Compound	Estimated Detection Limit[a]	
		ng/m^3	ppt
Halogenated hydrocarbon	Vinyl bromide	250	57
	Bromoform	0.340	0.03
	Bromodichloromethane	1.300	0.22
	Dibromochloromethane	0.667	0.07
	1-Bromo-2-chloroethane	1.00	0.67
	Allyl bromide	5.00	1.04
	1-Bromopropane	5.200	1.06
	1-Chloro-3-bromopropane	0.150	0.01
	1-Chloro-2,3-dibromopropane	~0.100	<0.01
	1,1-Dibromo-2-chloropropane	~0.100	<0.01
	1,2-Dibromoethane	0.530	0.07
	1,3-Dibromopropane	~0.100	~0.01
	Epichlorohydrin (1-Chloro-2,3-epoxypropane)	9.600	2.50
	Epibromohydrin (1-Bromo-2,3-epoxypropane)	0.300	0.05
	Bromobenzene	0.100	0.02
	Methyl bromide	500	135
	Methyl chloride	2000	1000
	Vinyl chloride	800	333
	Methylene chloride	700	200
	Chloroform	200	420
	Carbon tetrachloride	250	400

(continued)

Table A1 (cont'd)

Chemical Class	Compound	Estimated Detection Limit[a] ng/m^3	Estimated Detection Limit[a] ppt
Halogenated hydrocarbon (cont'd)	1,2-Dichloroethane	32	8.15
	1,1,1-Trichloroethane	66	12.45
	Tetrachloroethylene	2.5	0.38
	Trichloroethylene	10	1.92
	1-Chloro-2-methylpropene	62	21.5
	3-Chloro-2-methylpropene	62	21.5
	3-Chloro-1-butene	83	28.8
	Allyl chloride	83	28.8
	4-Chloro-1-butene	38	13.2
	1-Chloro-2-butene	13	4.5
	Chlorobenzene	2.10	0.47
	o-Dichlorobenzene	1.00	0.06
	m-Dichlorobenzene	0.75	0.01
	Benzylchloride	0.65	0.01
Halogenated ethers	2-Chloroethyl ethyl ether	4.15	0.97
	Bis-(chloromethyl)ether	1.0	1.10
Nitrosamines	N-Nitrosodimethylamine	5.0	1.67
	N-Nitrosodiethylamine	3.0	0.74
Oxygenated hydrocarbons	Acrolein	~100	56.5
	Glycidaldehyde	~59	9.5
	Propylene oxide	~60	25.5

(continued)

Table Al (cont'd)

Chemical Class	Compound	Estimated Detection Limit[a]	
		ng/m^3	ppt
Oxygenated hydrocarbons (cont'd)	Butadiene diepoxide	~20	6.7
	Cyclohexene oxide	~10	2.5
	Styrene oxide	2	0.415
	Acetophenone	~2	~0.415
	β-Propiolactone	~3	~1.2
Nitrogenous Compounds	Nitromethane	8	~2.4
	Aniline	3.0	0.78
Sulfur Compounds	Diethyl sulfate	~50	-
	Ethyl methane sulfate	~5.0	-

[a] Limits are calculated on the basis of the breakthrough volume for 2.2 g of Tenax GC, (at 70°F), capillary column performance and sensitivity of the mass spectrometer to that compound in the mass fragmentography mode of most intense ion.

there are 53 isomers. As the number of carbon atoms increases in the hydrocarbons and aromatics, the number of potential isomers becomes increasingly large and difficult to completely resolve by gas chromatography and/or by their corresponding mass cracking patterns. However, differentiation between the hydrocarbons, that is alkanes, alkenes, aromatics, oxygenated, etc. can be accomplished.

4.0 Reproducibility

The reproducibility of this method has been determined to range from ±10 to ±30% of the relative standard deviation for different substances when replicate sampling cartridges are examined (5). The inherent analytical errors are a function of several factors: [1] the ability to accurately determine the breakthrough volume for each of the identified organic compounds, [2] the accurate measurement of the ambient air volume sampled, [3] the percent recovery of the organic from the sampling cartridge after a period of storage, [4] the reproducibility of thermal desorption for a compound from the cartridge and its introduction into the analytical system, [5] the accuracy of determining the relative molar response ratios between the identified substance and the external standard used for calibrating the analytical system, [6] the reproducibility of transmitting the sample through the high resolution gas chromatographic column and, [7] the day-to-day reliability of the ms/comp system (1-8).

The accuracy of analysis is generally ±30% but depends on the chemical and physical nature of the compound (2,8).

5.0 Advantages and Disadvantages of the Method

The gas chromatograph/mass spectrometer interfaced with a glass jet separator, is extremely sensitive and specific for the analysis of many volatile organic compounds in ambient air. High resolution gas chromatographic separation provides adequate resolution of the substances found in ambient air for their subsequent quantification. The combination of the high resolution gas chromatographic column and the selection of specific or unique ions representing the various compounds of interest identified in the air samples yields a relatively specific assay method for these compounds (1-8).

Collected samples can be stored up to one month with less than 10% losses for most of the chemical classes (2,8). Because some of the compounds of interest may be hazardous to man, it is extremely important to exercise safety precautions in the preparation and disposal of liquid and gas standards, cleaning of used glassware, etc. in the analysis of air samples.

Since the mass spectrometer cannot be conveniently mobilized, sampling must be carried out away from the instrument.

The efficiency of air sampling increases as the ambient air decreases (i.e., sensitivity increases) (8).

The retention of water by Tenax is low; its thermal stability is high; and its background is negligible allowing sensitivity analysis (1,2,5,8).

6.0 Apparatus

6.1 Sampling Cartridges

The sampling tubes are prepared by packing a ten centimeter long by 1.5 cm i.d. glass tube containing 6 cm of 35/60 mesh Tenax GC with glass wool in the ends to provide support (2,5). Virgin Tenax (or material to be recycled) is extracted in a Soxhlet apparatus for a minimum of 18 hours each time with acetone and hexane prior to preparation of cartridge samplers (2,5). After purification of the Tenax GC sorbent and drying in a vacuum oven at 100°C for 3 to 5 hours at 28 inches of water, all the sorbent material is meshed to provide a 35/60 particle size range. Cartridge samplers are then prepared and conditioned at 270°C with helium flow at 30 ml/min for 30 min. The conditioned cartridges are transferred to Kimax® (2.5 cm x 150 cm) culture tubes immediately sealed using Teflon-lined caps and cooled. This procedure is performed in order to avoid recontamination of the sorbent bed (2,5).

Cartridge samplers with longer beds of sorbent may be prepared using a proportionally increased amount of Tenax in order to achieve a larger breakthrough volume for compounds of interest, and thus increasing the overall sensitivity of the technique (8).

6.2 Gas Chromatographic Column

A 0.35 mm i.d. x 100 m glass SCOT capillary column coated with SE-30 stationary phase and 0.1% benzyltriphenylphosphonium chloride is used for effecting the resolution of the volatile organic compounds (5). The capillary volume is conditioned for 48 hrs. at 245° at 2.25 ml/min of helium flow.

A glass jet separator on a Varian MAT CH-7 gc/ms/comp system is employed to interface the glass capillary column to the mass spectrometer. The glass jet separator is maintained at 240°C (2,5).

6.3 Inlet Manifold

An inlet manifold for thermally recovering vapors trapped on Tenax sampling cartridges is used and is shown in Figure A1 (1,2,4,5).

6.4 Gas Chromatograph

A Varian 1700 gas chromatograph is used to house the glass capillary column and is interfaced to the inlet manifold (Figure A1).

6.5 Mass Spectrometry/Computer

A Varian MAT CH-7 mass spectrometer with a resolution of 2,000 equipped with a single ion monitoring capability is used in tandem with a gas chromatograph (Figure A1). The mass spectrometer is interfaced to a Varian 620/L computer (Figure A1).

7.0 Reagents and Materials

All reagents used are analytical reagent grade.

8.0 Procedure

8.1 Cleaning of Glassware

All glassware, sampling tubes, cartridge holders, etc. are washed in Isoclean/water, rinsed with deionized distilled water, acetone and air dried. Glassware is heated to 450-500°C for 2 hours to insure that all organic material has been removed prior to its use.

8.2 Preparation of Tenax GC

Virgin Tenax GC is extracted in a Soxhlet apparatus for a minimum of 18 hours with acetone or methanol prior to its use. The Tenax GC sorbent is dried in a vacuum oven at 100°C for 3-5 hours and then sieved to provide a fraction corresponding to 35/60 mesh. This fraction is used for preparing sampling cartridges. In those cases where sampling cartridges of Tenax GC are recycled, the sorbent is extracted in a Soxhlet apparatus with acetone or methanol as described for the virgin material, but the sorbent is further extracted with a non-polar solvent, hexane, in order to remove the relatively non-polar and non-volatile materials which might have accumulated on the sorbent bed during previous sampling periods.

8.3 Collection of Volatile Organics in Ambient Air

Continuous sampling of ambient air is accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Figure A1, Reference 2). Flow rates between 1-10 ℓ/min are available with this sampling system. Flow rates are generally maintained at 1 ℓ using critical orifices and the total flow is monitored through a calibrated flow meter. The total flow is also registered by a dry gas meter. Con-concomitant with these parameters the temperature is continuously recorded with a Meterological Research, Inc. Weather Station since the breakthrough volume is important in order to obtain quantitative data on the volatile organics. This portable sampling unit operates on a 12 volt storage battery and is capable of continuous operation up to a period of 24 hours. However, in most cases at the rates which are employed in the field, the sampling period is generally 1-3 hours. This portable sampling unit is generally utilized for obtaining "high volume" samples. Duplicate cartridges are deployed on each sampling unit utilizing a sampling head as shown in Figure A2.

In addition to the Nutech samplers, DuPont personnel samplers are also used to acquire "low volumes" of ambient air as well as long-term integrated samples (12-36 hrs). Identical Tenax GC sampling cartridges are employed in this case, and the sampling is conducted in duplicate. The flow rate is balanced between duplicate cartridges using critical orifices to maintain a rate of 25-100 ml/min per cartridge.

For large sample volumes, it is important to realize that a total volume of air may cause the elution of compounds through the sampling tube if their breakthrough volume is exceeded. The breakthrough volumes of some of the volatile organics are shown in Table A2 (2,4,7,8). These breakthrough volumes have been determined by a previously described technique (2). The breakthrough volume is defined as that point at which 50% of a discrete sample introduced into the cartridge is lost. Although the identity of a compound during ambient air sampling is not known (therefore, also its breakthrough volume), the compound can still be quantified after identification by gc/ms/comp once the breakthrough

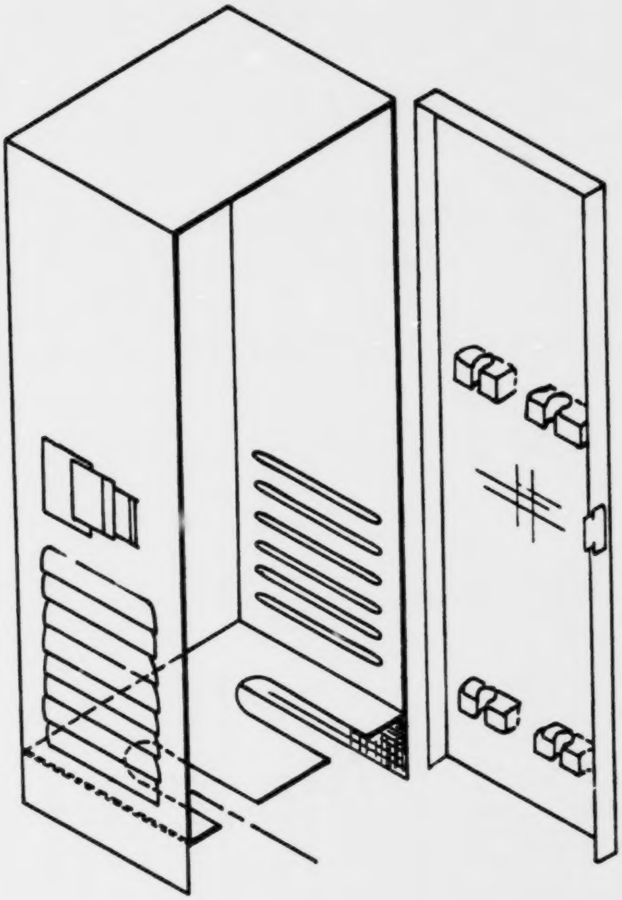


Figure A2. Sampling head for housing cartridge sampling train.

Table A2. TENAX GC BREAKTHROUGH VOLUMES FOR SEVERAL ATMOSPHERIC POLLUTANTS[1]

Chemical Class	Compound	b.p. (°C)	Temperature (°F)					
			50	60	70	80	90	100
Halogenated hydrocarbon	methyl chloride	-24	8	6	5	4	3	2.5
	methyl bromide	3.5	3	2	2	1	1	0.9
	vinyl chloride	13	2	1.5	1.25	1.0	0.8	0.6
	methylene chloride	41	11	9	7	5	4	3
	chloroform	61	42	31	24	18	13	10
	carbon tetrachloride	77	34	27	21	16	13	10
	1,2-dichloroethane	83	53	41	31	23	18	14
	1,1,1-trichloroethane	75	23	18	15	12	9	7
	tetrachloroethylene	121	361	267	196	144	106	78
	trichloroethylene	87	90	67	50	38	28	21
	1-chloro-2-methylpropene	68	26	20	16	12	9	7
	3-chloro-2-methylpropene	72	29	22	17	13	10	8
	1,2-dichloropropane	95	229	162	115	81	58	41
	1,3-dichloropropane	121	348	253	184	134	97	70
	epichlorohydrin (1-chloro-2,3-epoxypropane)	116	200	144	104	74	54	39
	3-chloro-1-butene	64	19	15	12	9	7	6
	allyl chloride	45	21	16	12	9	6	5
	4-chloro-1-butene	75	47	36	27	20	15	12
	1-chloro-2-butene	84	146	106	77	56	40	29
	chlorobenzene	132	899	653	473	344	249	181
	o-dichlorobenzene	181	1,531	1,153	867	656	494	372
	m-dichlorobenzene	173	2,393	1,758	1,291	948	697	510

(continued)

Table A2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F) 50	60	70	80	90	100
Halogenated hydrocarbons (cont'd)	benzyl chloride	179	2,792	2,061	1,520	1,125	830	612
	bromoform	149	507	386	294	224	171	131
	ethylene dibromide	131	348	255	188	138	101	74
	bromobenzene	155	2,144	1,521	1,079	764	542	384
Halogenated Ethers	2-chloroethyl ethyl ether	108	468	336	241	234	124	89
	Bis-(chloromethyl)ether	-	995	674	456	309	209	142
Nitrosamines	N-nitrosodimethylamine	151	385	280	204	163	148	107
	N-nitrosodiethylamine	177	2,529	1,836	1,330	966	700	508
Oxygenated hydrocarbons	acrolein	53	19	14	10	8	6	4
	glycidaldehyde	-	364	247	168	114	77	52
	propylene oxide	34	35	24	17	11	8	5
	butadiene diepoxide	-	1,426	1,009	714	506	358	253
	cyclohexene oxide	132	2,339	1,644	1,153	811	570	400
	styrene oxide	194	5,370	3,926	2,870	2,094	1,531	1,119
	phenol	183	2,071	1,490	1,072	769	554	398
	acetopheonone	202	3,191	2,382	1,778	1,327	991	740
	β-propiolactone	57	721	514	366	261	186	132
Nitrogenous Hydrocarbons	nitromethane	101	45	34	25	19	14	11
	aniline	184	3,864	2,831	2,075	1,520	1,114	817
Sulfur Compounds	diethyl sulfate	208	40	29	21	15	11	8
	ethyl methane sulfate	86	5,093	3,681	2,564	1,914	1,384	998

(continued)

Table A2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F)					
			50	60	70	80	90	100
Amines	dimethylamine	7.4	9	6	4	3	2	1
	isobutylamine	69	71	47	34	23	16	11
	t-butylamine	89	6	5	4	3	2	1
	di-(*n*-butyl)amine	159	9,506	7,096	4,775	3,105	2,168	1,462
	pyridine	115	378	267	189	134	95	67
	aniline	184	8,128	5,559	3,793	2,588	1,766	1,205
Ethers	diethyl ether	34.6	29	21	15	11	8	5
	propylene oxide	35	13	9	7	5	4	3
Esters	ethyl acetate	77	162	108	72	48	32	22
	methyl acrylate	80	164	111	75	50	34	23
	methyl methacrylate	100	736	484	318	209	137	90
Ketones	acetone	56	25	17	12	8	6	4
	methyl ethyl ketone	80-2	82	57	39	27	19	13
	methyl vinyl ketone	81	84	58	40	28	19	14
	acetophenone	202	5,346	3,855	2,767	2,000	1,439	1,037
Aldehydes	acetaldehyde	20	3	2	2	1	0.9	0.7
	benzaldehyde	179	7,586	5,152	3,507	2,382	1,622	1,101
Alcohols	methanol	64.7	1	1	0.8	0.6	0.4	0.3
	n-propanol	97.4	27	20	14	10	7	5
	allyl alcohol	97	32	23	16	11	8	6

(continued)

Table A2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F) 50	60	70	80	90	100
Aromatics	benzene	80.1	108	77	54	38	27	19
	toluene	110.6	494	348	245	173	122	86
	ethylbenzene	136.2	1,393	984	693	487	344	243
	cumene	152.4	3,076	2,163	1,525	1,067	750	527
Hydrocarbons	*n*-hexane	68.7	32	23	17	12	9	6
	n-heptane	98.4	143	104	75	55	39	29
	1-hexene	63.5	28	20	15	11	8	6
	1-heptene	93.6	286	196	135	93	64	44
	2,2-dimethylbutane	49.7	0.5	0.4	0.3	0.2	0.2	0.1
	2,4-dimethylpentane	80.5	435	252	146	84	49	28
	4-methyl-1-pentene	53.8	14	10	8	6	4	3
	cyclohexane	80.7	49	36	26	19	14	10
Inorganic gases	nitric oxide	-	0	0	0	0	0	0
	nitrogen dioxide	-	0	0	0	0	0	0
	chlorine	-	0	0	0	0	0	0
	sulfur dioxide	-	0.06	0.05	0.03	0.02	0.02	0.01
	water	100	0.06	0.05	0.04	0.03	0.01	0

[a] Breakthrough volume is given in ℓ/2.2 g Tenax GC used in sampling cartridges.

volume has subsequently been established. Thus, the last portion of the sampling period is selected which represents the volume of air sampled prior to breakthrough for calculating their concentration. For cases in which the identity of a volatile organic compound is not known until after glc/ms, the breakthrough volume is subsequently determined.

Previous experiments have shown that the organic vapors collected on Tenax GC sorbent are stable and can be quantitatively recovered from the cartridge samplers up to 4 weeks after sampling when they are tightly closed in cartridge holders and placed in a second container that can be sealed, protected from light and stored at 0°C (1,2).

8.4 Analysis of Samples

The instrumental conditions for the analysis of volatile organics on the sorbent Tenax GC sampling cartridge is shown in Table A3. The thermal desorption chamber and the six port valco valve are maintained at 270° and 240°, respectively. The glass jet separator is maintained at 240°. The mass spectrometer is set to scan the mass range from 25-350. The helium purge gas through the desorption chamber is adjusted to 15-20 ml/min. The nickel capillary trap on the inlet manifold is cooled with liquid nitrogen. In a typical thermal desorption cycle, a sampling cartridge is placed in the preheated desorption chamber and the helium gas is channeled through the cartridge to purge the vapors into the liquid nitrogen capillary trap [the inert activity of the trap has been shown in a previous study (5)]. After the desorption has been completed, the six-port valve is rotated and the temperature on the capillary loop is rapidly raised (greater than 10°/min); the carrier gas then introduces the vapors onto the high resolution gc column. The glass capillary column is temperature programmed from ambient to 240°C at 4°C/min and held at the upper limit for a minimum of 10 min. After all the components have been eluted from the capillary column, the analytical column is then cooled to ambient temperature and the next sample is processed (2).

An example of the analysis of volatile organics in ambient air is shown in Figure A3 and the background from a blank cartridge is shown in Figure A4. The high resolution glass capillary column was coated with SE-30 stationary which is capable of resolving a multitude of compounds

Table A3. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC	
100 m glass SCOT-SE/30	25-240°C, 4°C/min
carrier (He) flow	∿3 ml/min
transfer line to ms	240°C
MS	
scan range	*m/e* 20 → 300
scan range, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	6.0
ion source vacuum	∿4 x 10^{-6} torr

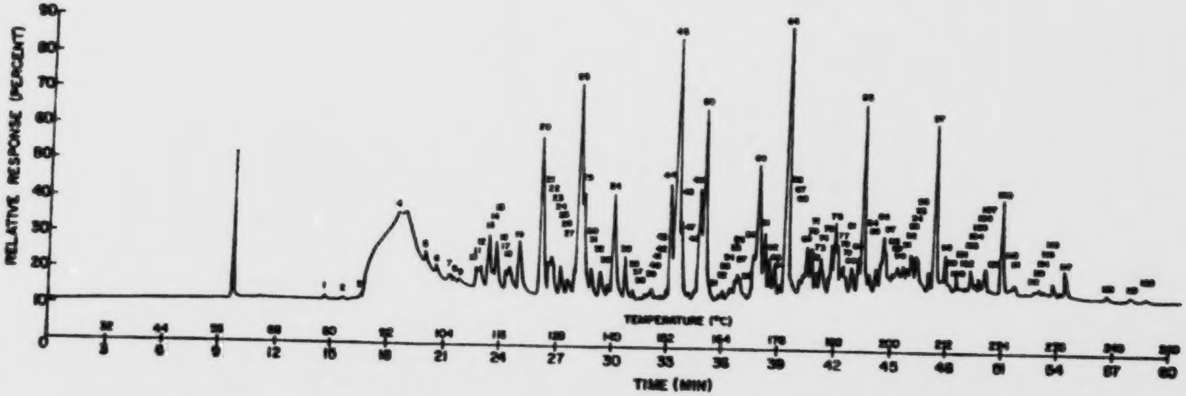


Figure A3. Profile of ambient air pollutants for Wood River, IL using high resolution gas chromatography/mass spectrometry/computer.

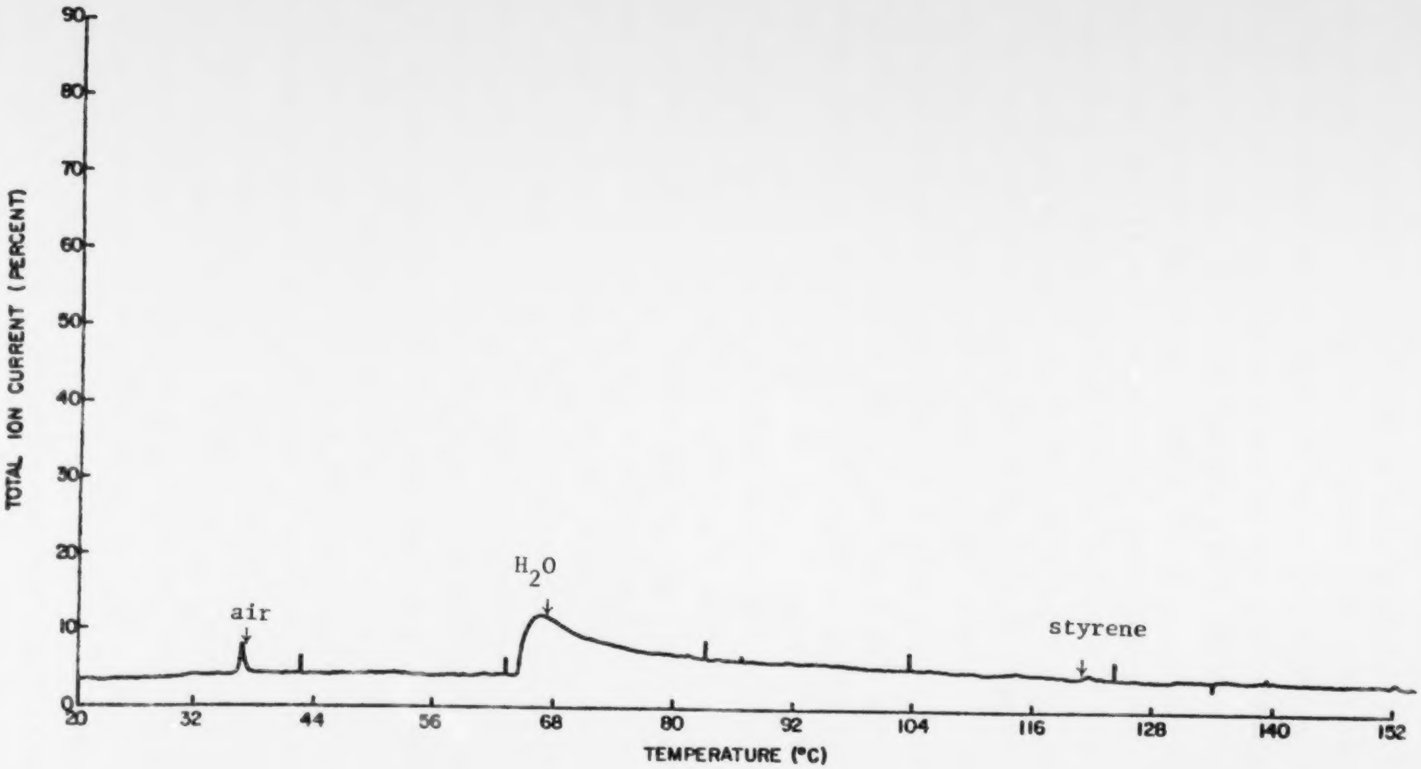


Figure A4. Background profile for Tenax GC cartridge blank.

to allow their subsequent identification by ms/comp techniques; in this case over 120 compounds were identified in this chromatograph.

8.4.1 Operation of the MS/COMP System (Figure A5)

Typically the mass spectrometer is first set to operate in the repetitive scanning mode. In this mode the magnet is automatically scanned exponentially upward from a preset low mass to a high mass value. Although the scan range may be varied depending on the particular sample, typically the range is set from m/e 25 to m/e 300. The scan is completed in approximately 1.8 seconds. At this time the instrument automatically resets itself to the low mass position in preparation for the next scan, and the information is accumulated by an on-line 620/L computer and written onto magnetic tapes or the dual disk system. The reset period requires approximately 2.0 seconds. Thus, a continuous scan cycle of 3.8 seconds/scan is maintained and repetitively executed throughout the chromatographic run. The results is the accumulation of a continuous series of mass spectra throughout the chromatographic run in sequential fashion.

Prior to running unknown samples, the system is calibrated by introducing a standard substance, perfluorokerosene, into the instrument and determining the time of appearance of the known standard peaks in relation to the scanning magnetic field. The calibration curve which is thus generated is stored in the 620/L computer memory. This calibration serves only to calibrate the mass ion over the mass scanning range.

While the magnet is continuously scanning, the sample is injected and automatic data acquisition is initiated. As each spectrum is acquired by the computer, each peak which exceeds a preset threshold is recognized and reduced to centroid time and peak intensity. This information is stored in the computer core while the scan is in progress. In addition, approximately 30 total ion current values and an equal number of Hall probe signals are stored in the core of the computer as they are acquired. During the two-second period between scans this spectral information, along with the spectrum number, is written sequentially on disks, and the computer is reset for the acquisition of the next spectrum.

This procedure continues until the entire gc run is completed. By this time there are from 800-1400 spectra on the disk which are then subsequently processed. Depending on the information required, that day

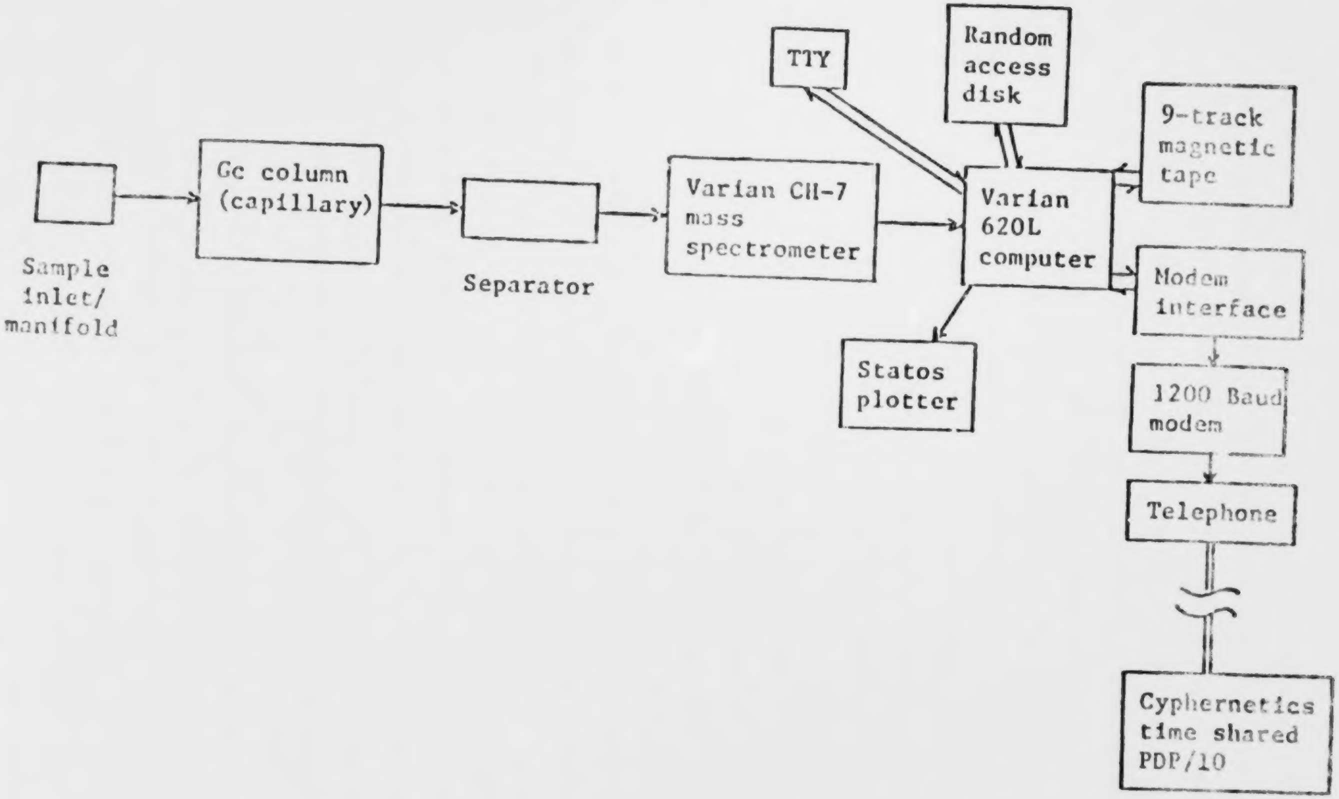

Sample
inlet/
manifold
Gc column
(capillary)
Separator
Varian CH-7
mass
spectrometer
TTY
Random
access
disk
Varian
620L
computer
9-track
magnetic
tape
Modem
interface
1200 Baud
modem
Telephone
Cyphernetics
time shared
PDP/10
Statos
plotter

Figure A5. Schematic diagram of gc-ms computer system.

may then either be processed immediately or additional samples may be run, stored on magnetic tape and the results examined at a later time.

The mass spectral data are processed in the following manner. First, the original spectra are scanned and the total ion current (TIC) information is extracted. Then the TIC intensities are plotted against the spectrum number on the Statos 31 recorder. The information will generally indicate whether the run is suitable for further processing, since it provides some idea of the number of unknowns in the sample and the resolution obtained using the particular gc column conditions.

The next stage of the processing involves the mass conversion of the spectral peak times to peak masses which is done directly via the dual disk system. The mass conversion is accomplished by use of the calibration table obtained previously using perfluorokerosene. Normally one set of the calibration data is sufficient for an entire day's data processing since the characteristics of the Hall probe are such that the variation in calibration is less than 0.2 atomic mass units/day. A typical time required for this conversion process for 1,000 spectra is approximately 30 min.

After the spectra are obtained in mass converted form, processing proceeds either manually or by computer. In the manual mode, the full spectrum of scans for the gc run is recorded on the Statos 31 plotter. The TIC information available at this time is most useful for deciding which spectra are to be analyzed. At the beginning of the runs where peaks are very sharp nearly every spectrum must be inspected individually to determine the identity of the component. Later in the chromatographic run when the peaks are broader only selected scans need to be analyzed.

Identification of resolved components is achieved by comparing the mass cracking patterns of the unknown mass spectra to an eight major peak index of mass spectra (9). Individual difficult unknowns are searched by the use of the Cornell University STIRS and PBM systems. Unknowns are also submitted to EPA MSSS system for identification. When feasible, the identification of unknowns are confirmed by comparing the cracking pattern and elution temperatures for two different chromatographic columns (SE-30 and Carbowax SCOT capillaries) for the unknown and authentic compounds. The relationship between the boiling point of the identified halogenated hydrocarbon and the elution temperature on a non-polar column (the order of elution of constituents is predictable in homologous series since the SE-30 SCOT capillary separates primarily on the basis of boiling point) is carefully considered in making structure assignments.

Mass spectral search programs are operational at the Triangle Universities Computation Center (TUCC). RTI maintains twice daily service to TUCC, which is a one-quarter mile distance from the RTI campus. Additional information about each magnetic tape containing the mass spectra of halogenated hydrocarbons is entered directly into the TUCC job stream using a remote job entry processing. This is normally done at TUCC using one of the five terminals located within the Analytical Sciences Laboratory. The control information contains selected spectrum numbers of instructions to process entire gc runs. The computer program systems compare simultaneously either the entire library of 25,000 compounds or some subset of this library. The complete reports showing the best fits for each of the unknowns is produced at TUCC and printed out at the high speed terminals located on the RTI campus of TUCC. Thus, the processing of the mass spectral data obtained for the halogenated hydrocarbons in the samples collected is processed by one of three routes. Each consists of a different level of effort. The first level is strictly a manual interpretation process which proves to be the most thorough approach. The second level is executed when the interpretation at the first level has not yielded conclusive results.

8.4.2 Quantitative Analysis

In many cases the estimation of the level of pollutants by capillary gas chromatography in combination with mass spectrometry is not feasible utilizing only the total ion current monitor (See Figure A3 for example). Since baseline resolution between peaks is not always achieved, we employ the techniques which have been previously developed under contract whereby full spectra are obtained during the chromatographic separation step and the selected ions are presented as mass fragmentograms using computer software programs which allow the possibility of deconvoluting constituents which were not resolved in the total ion current chromatogram (6). Examples are depicted in Figures A6 and A7 which represent an ambient air sample with a TIC profile as in Figure A3.

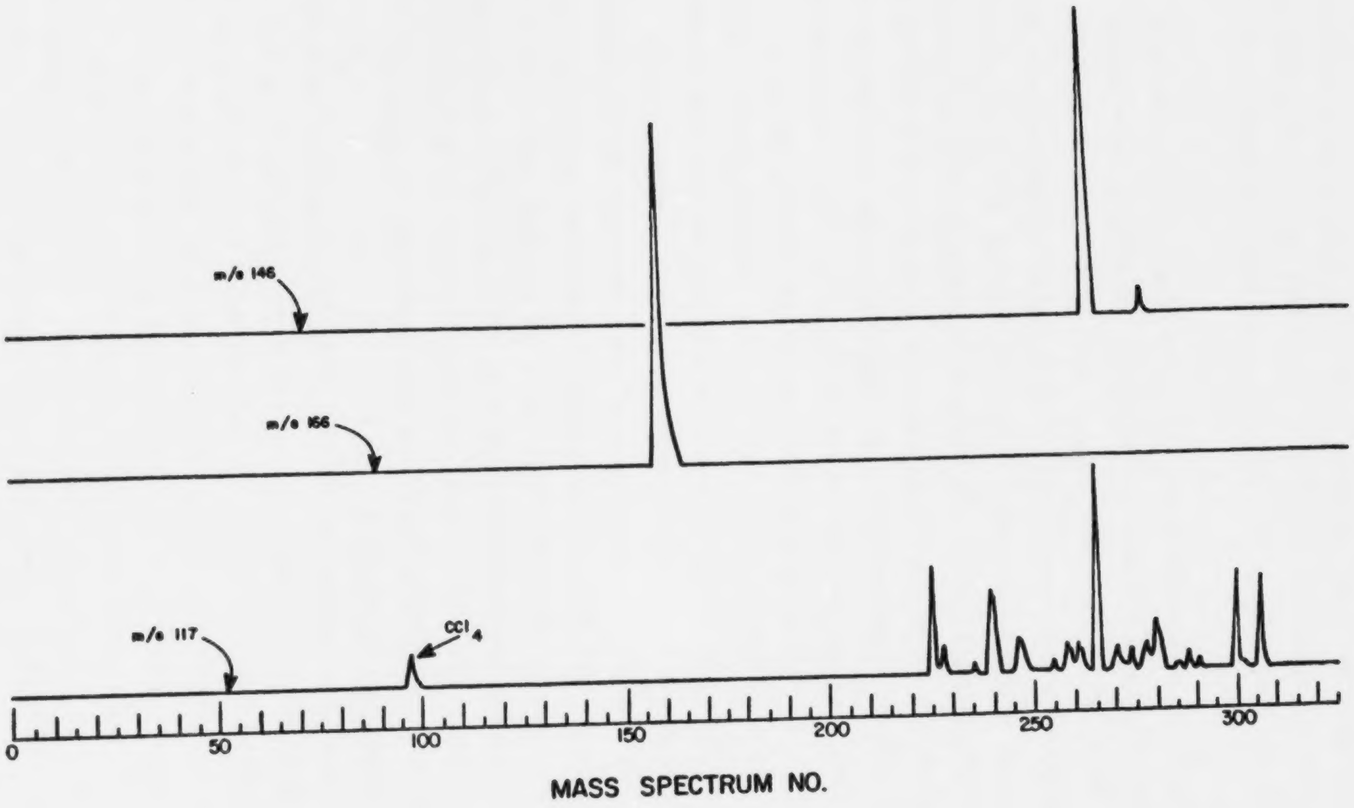


Figure A6. Mass fragmentograms of characteristic ions representing carbon tetrachloride (m/e 117), tetrachloroethylene (m/e 166) and m-dichlorobenzene (m/e 146) in ambient air.

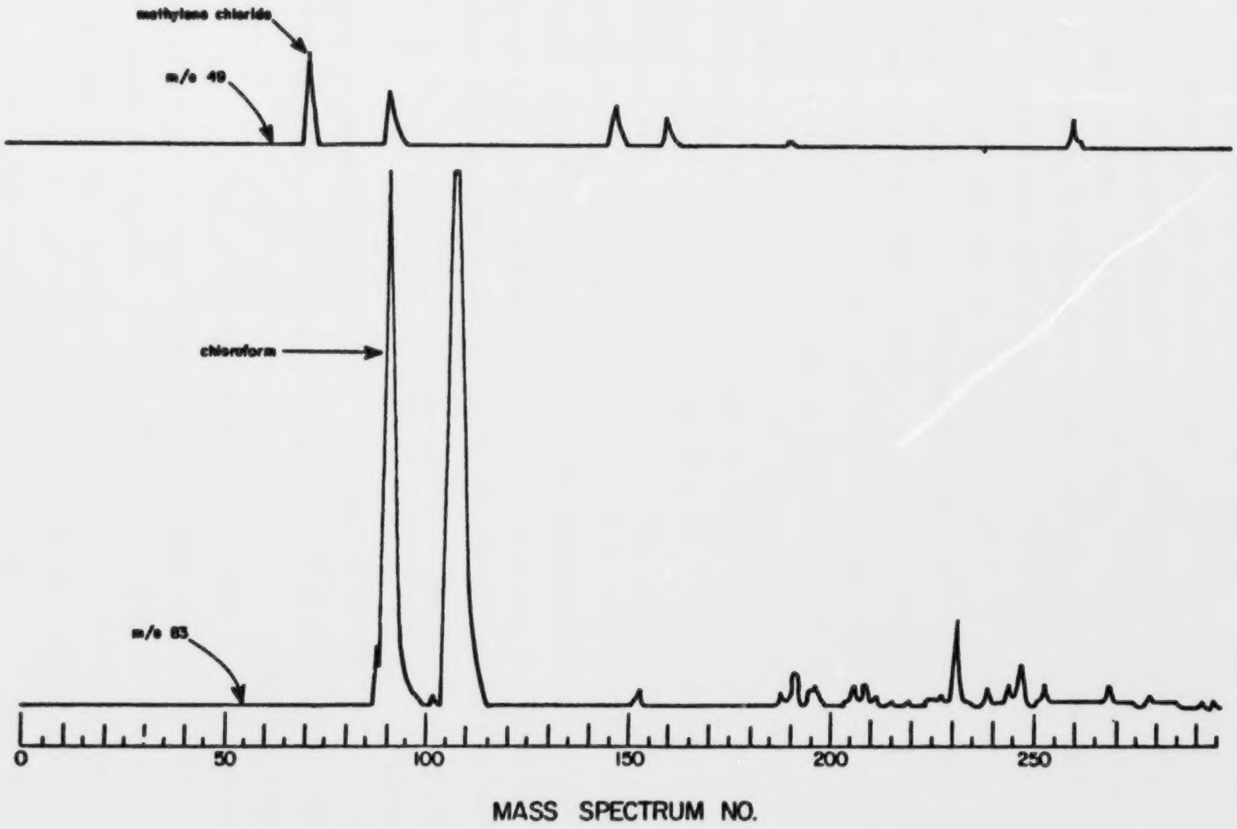


Figure A7. Mass fragmentograms of characteristic ions representing methylene chloride (m/e 49) and chloroform (m/e 83) in ambient air.

The standard added can be added as an internal standard during sampling, however, since the volume of air taken to produce a given sample is accurately known, it is also possible and more practical to use an external standard whereby the standard is introduced into the cartridge prior to its analysis. Two standards, hexafluorobenzene and perfluorotoluene are used for the purpose of calculating RMR's. From previous research it has been determined that the retention times for these two compounds are such that they elute from the glass capillary column (SE-30) at a temperature and retention time which does not interfere with the analysis of unknown compounds in ambient air samples.

Since the volume of air taken to produce a given sample is accurately known and an external standard is added to the sample, then the weight can be determined per cartridge and hence the concentration of the unknown. The approach for quantitating ambient air pollutants requires that the RMR is determined for each constituent of interest. This means that when an ambient air sample is taken, the external standard is added during the analysis at a known concentration. It is not imperative at this point to know what the RMR of each of the constituents in the sample happens to be. However, after the unknowns are identified then the RMR can be subsequently determined and the unknown concentration calculated in the original sample using the RMR. In this manner it is possible to obtain qualitative and quantitative information on the same sample with a minimum of effort.

9.0 References

1. Pellizzari, E. D., Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres. Publication No. EPA-650/2-74-121, Contract No. 68-02-1228, 148 pp., July, 1974.
2. Pellizzari, E. D., Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. Publication No. EPA-600/2-75-075, Contract No. 68-02-1228, 187 pp., November, 1975.
3. Pellizzari, E. D., J. E. Bunch, B. H. Carpenter and E. Sawicki, Environ. Sci. Tech., 9, 552 (1975).
4. Pellizzari, E. D., B. H. Carpenter, J. E. Bunch and E. Sawicki, Environ. Sci. Tech., 9, 556 (1975).

5. Pellizzari, E. D., The Measurement of Carcinogenic Vapors in Ambient Atmospheres. Publication No. EPA-600/7-77-055, Contract No. 68-02-1228, 288 pp., June, 1977.
6. Pellizzari, E. D., J. E. Bunch, R. E. Berkley and J. McRae, Anal. Chem., 48, 803 (1976).
7. Pellizzari, E. D., Quarterly Report No. 1, EPA Contract No. 68-02-2262, February, 1976.
8. Pellizzari, E. D., J. E. Bunch, R. E. Berkley and J. McRae, Anal. Lett., 9, 45 (1976).
9. "Eight Peak Index of Mass Spectra", Vol. 1, (Tables 1 and 2) and II (Table 3), Mass Spectrometry Data Centre, AWRE, Aldermaston, Reading, RF74PR, UF, 1970.
10. Pellizzari, E. D., Quarterly Report No. 3, EPA Contract No. 68-02-2262, in preparation.
11. Pellizzari, E. D., "Measurement of Carcinogenic Vapors in Ambient Atmospheres", EPA Contract No. 68-02-1228, Final Report, in press.

Written analytical protocol prepared 1/24/77.

APPENDIX B

VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR

Part I	Iberville Parish and Baton Rouge, LA
Part II	Linden and Deepwater, NJ
Part III	Camden, NJ-Philadelphia, PA

Part I

Iberville Parish and Baton Rouge, LA

Table B1. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH IN LOUISIANA[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound	MS No.
1	43	$N_2 + O_2$	140
2	43	CO_2	145
3	45	dichlorodifluoromethane (freon 12)	149
4	46	C_4H_8 isomer	152
5	48	C_4H_{10} isomer	155
6	52	C_5H_{12} isomer	163
7	53	trichlorofluoromethane	165
8	55	C_5H_{12} isomer	168
9	55	acetaldehyde	171
10	57	CS_2	175
11	57	methylene chloride	175
12	62	C_6H_{14} isomer	183
13	64	C_6H_{14} isomer	187
14	66	perfluorobenzene (std.)	190
15	66	C_6H_{14} isomer	192
16	68	chloroform	195
17	71	perfluorotoluene (std.)	200
18	74	1,1,1-trichloroethane	205
19	76	1,2-dichloroethane	209
20	76	benzene	210
21	76	carbon tetrachloride	210
22	77	cyclohexane	212
23	78	C_7H_{16} isomer	214
24	80	C_7H_{16} isomer	218
25	80	C_7H_{14} isomer	220
26	82	C_8H_{18} isomer	222
27	83	C_7H_{16} isomer	226
28	84	dichlorobutane	229
29	88	C_7H_{14} isomer	235
30	90	C_8H_{16} isomer	239
31	90	C_8H_{18} isomer	239
32	93	C_8H_{18} isomer	246
33	95	C_8H_{18} isomer	248
34	97	toluene	251
35	97	C_8H_{18} isomer	252
36	98	C_8H_{16} isomer	257
37	102	C_8H_{18} isomer	265
38	105	tetrachloroethylene	268
39	110	C_9H_{18} isomer	280
40	114	ethylbenzene	288
41	116	m- and/or p-xylene	291
42	120	o-xylene	300
43	120	C_9H_{18} isomer	300
44	123	C_9H_{20} isomer	303
45	126	C_3-alkyl benzene	311
46	134	C_3-alkyl benzene	327
47	136	C_3-alkyl benzene	331
48	139	C_3-alkyl benzene	337
49	140	$C_{10}H_{22}$ isomer	339
50	141	benzaldehyde	340
51	150	C_4-alkyl benzene	356
52	154	C_4-alkyl benzene	365
53	157	$C_{11}H_{24}$ isomer	374
54	157	acetophenone	374
55	160	C_4-alkyl benzene	380
56	172	C_2-alkyl phenol	401
57	176	C_2-alkyl phenol	410
58	214	$C_{15}H_{28}$ isomer	488
59	215	$C_{15}H_{32}$ isomer	490
60	220	C_5-alkyl benzene	500
61	225	phenyl butyl ether	507
62	228	unknown	515
63	232	$C_{14}H_{28}$	524
64	240	alkyl phenyl ether	572

---

[a] See Table 27 for sampling protocol and Fig. 11 (L2) for sampling location.

Table B2. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH IN LOUISIANA[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
2A	45	chloromethane
3	47	1-butene + n-butane
4	51	isopentane
4B	52	C_5H_{10} isomer
4C	53	n-pentane
5	53	acetaldehyde
5A	54	C_5H_{10} isomer
5B	55	dichloromethane
5C	57	propanal
5D	57	propenal
6	59	2-methylpentane
6A	61	dimethyl ether
7	61	3-methylpentane
7A	62	acetone
8	63	hexafluorobenzene (eS)
8A	64	n-hexane
9	65	chloroform
9A	66	C_4H_8O isomer
10	68	perfluorotoluene (eS)
10A	68	methylcyclopentane (tent.)
10B	70	n-butanal
10C	71	1,1,1-trichloroethane
10D	72	1,2-dichloroethane
11	73	benzene + carbon tetrachloride
11A	74	cyclohexane
12	75	2-methylhexane
13	77	3-methylhexane
13A	78	C_7H_{14} isomer
14	79	C_8H_{18} isomer
14A	80	1,2-dichloropropane (tent.)
15	81	n-heptane
16	86	methylcyclohexane
17	88	C_8H_{18} isomer
17A	91	C_8H_{18} isomer
17B	92	C_8H_{18} isomer
18	94	toluene
19	96	C_8H_{18} isomer
20	97	C_8H_{16} isomer
20A	100	C_8H_{16} isomer
21	101	n-octane
21A	102	C_8H_{16} isomer
22	103	tetrachloroethylene
22A	104	C_9H_{20} isomer
22B	106	C_9H_{20} isomer
23	108	ethylcyclohexane
23A	109	C_9H_{18} isomer
23B	113	ethylbenzene
23C	114	C_9H_{20} isomer
24	115	p-xylene
24A	115	C_9H_{20} isomer
24B	117	C_9H_{20} isomer
24C	118	C_9H_{18} isomer
25	119	o-xylene
26A	120	styrene
26	121	n-nonane
27	125	$C_{10}H_{22}$ isomer
27A	127	$C_{10}H_{20}$ isomer (tent.)
28	128	$C_{10}H_{22}$ isomer
28A	131	n-propylbenzene
28B	132	p-ethyltoluene
29	133	$C_{10}H_{22}$ isomer
30	135	C_3-alkyl benzene + $C_{10}H_{22}$ isomers
31	138	C_3-alkyl benzene isomer
31A	139	benzaldehyde
32	139	n-decane
32A	143	$C_{11}H_{22}$ + C_3-alkyl benzene isomers
33	144	$C_{11}H_{24}$ isomer
33A	147	$C_{12}H_{26}$ isomer
33B	148	C_4-alkyl benzene isomer
34	149	C_4-alkyl benzene isomer
34A	149	$C_{11}H_{22}$ isomer
34B	150	$C_{11}H_{24}$ isomer
34C	153	C_4-alkyl benzene isomer
34D	154	$C_{10}H_{12}$ isomer
34E	155	acetophenone + $C_{11}H_{22}$ isomer
35	157	n-undecane
35A	159	$C_{12}H_{24}$ isomer
35B	161	$C_{12}H_{26}$ isomer
35C	164	cresol isomer
35D	167	C_2-alkyl phenol
35E	170	C_2-alkyl phenol
36	171	naphthalene + $C_{13}H_{26}$ isomer
37	173	n-dodecane
38	186	$C_{11}H_{22}O$ isomer
39	187	n-tridecane
39A	188	$C_{13}H_{26}$ isomer
40	202	n-tetradecane
40A	203	$C_{14}H_{28}$ isomer
41	210	$C_{15}H_{32}$ isomer

(continued)

Table B2 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
42	214	$C_{15}H_{30}$ isomer
43	215	*n*-pentadecane
44	218	tripropylene glycol methyl ether
45	226	$C_{16}H_{32}$ isomer
46	227	*n*-hexadecane
48	237	$C_{17}H_{34}$ isomer
49	239	$C_{17}H_{34}$ isomer
49A	240	$C_{17}H_{36}$ isomer

[a] See Table 27 for sampling protocol and Fig. 11 (L4) for sampling location.

Table B3. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH, LOUISIANA[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
3	48	*n*-butane + 1-butene
3A	49	C_4H_8 isomer + 2-butene
4	52	isopentane
4A	54	C_5H_{10} isomer
5	55	*n*-pentane
5A	55	acetaldehyde
6	57	C_6H_{14} isomer
6A	58	methylene chloride
6B	58	C_5H_{10} isomer
6C	60	*n*-propanal
6D	61	C_5H_{10} isomer
7	62	C_6H_{14} isomer
8	64	3-methylpentane
8A	65	C_6H_{12} isomer
9	66	perfluorobenzene (e[illegible])
9A	66	*n*-hexane
10	68	chloroform
11	70	perfluorotoluene (e[illegible])
11A	73	1,1,1-trichloroethane
11B	75	1,2-dichloroethane
12	76	benzene + CCl_4
12A	76	C_6H_{12} isomer
13	77	2-methylhexane
13A	78	C_7H_{16} isomer
14	79	C_7H_{16} isomer
14A	80	C_7H_{14} isomer
15	81	C_8H_{18} isomer
15A	82	1,2-dichloropropane
15B	83	trichloroethylene (tent.)
16	83	*n*-heptane
16A	85	C_7H_{14} isomer
17	87	C_7H_{14} isomer
18	89	C_8H_{18} isomer
18A	91	C_8H_{16} isomer
19	93	C_8H_{18} + C_8H_{16} isomer
19A	94	C_8H_{16} isomer
20	95	toluene
20A	96	C_8H_{18} isomer
21	96	C_8H_{18} isomer
21A	97	C_8H_{16} isomer
22	97	C_9H_{20} isomer
23	99	C_8H_{16} isomer
24	102	*n*-octane
25	104	tetrachloroethylene
25A	108	C_9H_{20} isomer
26	109	C_8H_{16} isomer
26A	109	C_9H_{20} isomer
26B	110	C_9H_{18} isomer
27	113	ethylbenzene
27A	114	C_9H_{18} isomer
28	115	xylene isomer
28A	116	C_9H_{20} isomer
29	116	$C_{10}H_{22}$ isomer
30	119	C_9H_{18} isomer
31	121	*n*-nonane
31B	122	C_9H_{18} isomer
31C	122	$C_{10}H_{22}$ isomer
31D	125	C_3-alkyl benzene isomer
31E	127	C_9H_{18} isomer
31F	128	$C_{10}H_{22}$ isomer
31G	128	*n*-propylbenzene
32	129	C_3-alkyl benzene isomer
33	131	$C_{10}H_{22}$ isomer
33A	131	C_3-alkyl benzene isomer
34	132	$C_{10}H_{22}$ isomer
35	133	C_3-alkyl benzene isomer
35A	133	$C_{10}H_{22}$ isomer
35B	134	$C_{10}H_{20}$ isomer
35C	135	$C_{10}H_{20}$ isomer
36	136	benzaldehyde + C_3-alkyl benzene isomer
37	137	*n*-decane
37A	140	C_4-alkyl benzene isomer
38	141	C_3-alkyl benzene isomer
38A	142	$C_{11}H_{24}$ isomer
38B	143	$C_{10}H_{20}$ isomer
38C	145	$C_{11}H_{24}$ isomer
38D	146	C_4-alkyl benzene isomer
39	146	C_4-alkyl benzene isomer
39A	148	$C_{11}H_{24}$ isomer
39B	148	C_4-alkyl benzene isomer
39C	150	C_4-alkyl benzene isomer
39D	151	C_4-alkyl benzene isomer
40	152	acetophenone
41	154	*n*-nonanal
41A	153	*n*-undecane
41C	155	$C_{11}H_{22}$ isomer
42	157	C_4-alkyl benzene isomer
42A	160	*p*-cresol
42B	161	$C_{11}H_{22}$ isomer
42C	162	*m*-cresol

(continued)

Table B3 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
42D	162	indan + methylstyrene isomer
42E	163	C_4-alkyl benzene isomer
42F	164	C_5-alkyl benzene isomer
42G	166	$C_{12}H_{26}$ + C_5-alkyl benzene isomer
42H	169	naphthalene
43	170	_n_-dodecane
43A	171	$C_{12}H_{24}$ isomer
43B	177	C_2-phenol isomer
44	211	_n_-pentadecane
44A	221	diethyl phthalate
45	225	_n_-hexadecane

[a] See Table 27 for sampling protocol and Fig. 11 (L5) for sampling location.

Table B4. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH, LOUISIANA[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	42	CO_2
2	43	chloroacetylene (tent.) + propylene
2A	45	propane + chloromethane
3	45	vinyl chloride
4	46	*n*-butane
4A	46	butadiene isomer
4B	47	C_4H_8 isomer
4C	48	chloroethane + C_5H_{10} isomer
4D	49	neopentane
5	49	isopentane
6	50	1-pentene
6A	51	*n*-pentane
7	51	acetaldehyde + isoprene
7A	52	vinylidene chloride + C_5H_{10} isomer
7B	52	propanal
8	53	dichloromethane
8A	54	C_5H_6 isomer + CS_2
8B	55	C_5H_8 isomer
8C	55	dimethyl ether
8D	56	cyclopentene
8E	56	acetone
9	57	2-methylpentene
9A	58	1,1-dichloroethane
10	59	3-methylpentene
10A	60	C_6H_{12} isomer
11	61	hexafluorobenzene (eS)
12	61	*n*-hexane
13	63	chloroform
14	65	perfluorotoluene (eS)
14A	66	methylcyclopentane
14B	67	*n*-butanal
15	67	1,2-dichloroethane
15A	68	1,1,1-trichloroethane (tent.)
16	71	benzene + carbon tetrachloride
16A	72	cyclohexane
17	73	2-methylhexane
17A	73	2,3-dimethylpentane
18	74	3-methylhexane
19	76	C_7H_{14} isomer
20	77	1,2-dichloropropane
20A	78	trichloroethylene
21	79	*n*-heptane
21A	79	dichloropropene isomer (tent.)
22	84	methylcyclohexane
22A	85	C_8H_{16} isomer
23	86	C_8H_{18} isomer
24	87	C_7H_{14} isomer (tent.)
25	90	C_8H_{18} isomer
26	91	1,1,2-trichloroethane
26A	92	toluene
26B	93	C_8H_{18} isomer
27	94	C_8H_{18} isomer
27A	96	C_8H_{16} isomer
27B	96	C_8H_{18} isomer
27C	98	C_8H_{16} isomer
28	100	*n*-octane
29	101	tetrachloroethylene
29A	107	C_2-alkyl cyclohexane isomer
30	108	C_9H_{20} isomer
30A	110	acetic acid (tent.)
30B	111	C_9H_{18} isomer
31	112	ethylbenzene
32	114	*p*-xylene
32A	115	C_9H_{20} isomer
33	118	*o*-xylene + styrene
33A	119	C_9H_{18} isomer
34	120	*n*-nonane
34A	124	$C_{10}H_{22}$ isomer
35	125	isopropylbenzene
35A	126	$C_7H_{14}O$ isomer (tent.)
35B	126	C_9H_{18} isomer
36	127	$C_{10}H_{22}$ isomer
36A	130	*n*-propylbenzene
36B	131	*m*-ethyltoluene
37	133	$C_{11}H_{24}$ isomer
37A	134	$C_{10}H_{22}$ isomer
38	135	C_3-alkyl benzene isomer
38A	136	$C_{10}H_{20}$ isomer
38B	137	$C_{10}H_{18}$ isomer
38C	137	$C_{10}H_{20}$ isomer
39	138	1,2,4-trimethylbenzene
39A	138	benzaldehyde
39B	139	$C_{10}H_{20}$ isomer
40	139	*n*-decane
40A	140	dichlorobenzene isomer (tent.)
41	143	1,2,3-trimethylbenzene
41A	143	$C_{11}H_{24}$ isomer
41B	144	$C_{11}H_{24}$ isomer + phenol
41C	146	C_4-alkyl cyclohexane isomer
42	147	bis-(2-chloroisopropyl)ether

(continued)

Table B4 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
42A	148	C_4-alkyl benzene isomer
42B	149	C_4-alkyl benzene isomer
42C	149	$C_{11}H_{22}$ isomer
42D	150	$C_{11}H_{24}$ isomer
42E	152	$C_{11}H_{22}$ isomer
42F	152	C_4-alkyl benzene isomer
42G	154	C_4-alkyl benzene isomer
42H	155	acetophenone + $C_{11}H_{22}$ isomer
42I	156	tetrachlorobutadiene isomer
43	157	n-undecane
43A	158	cresol isomer
43B	159	C_4-alkyl benzene isomer
44	164	dimethylphenol isomer
45	167	dimethylphenol isomer
46	171	naphthalene
46A	172	$C_{12}H_{24}$ isomer
47	173	n-dodecane
48	176	1,3-hexachlorobutadiene
49	180	tripropylene glycol
49A	181	C_3-alkyl phenol isomer
49B	185	C_3-alkyl phenol isomer
49C	187	$C_{13}H_{26}$ isomer
50	188	n-tridecane
50A	189	methylnaphthalene isomer
51	191	unknown
52	198	isobutyl isobutyrate
53	202	n-tetradecane
53A	214	$C_{13}H_{26}O$ isomer
54	215	$C_{15}H_{30}$ isomer
55	216	n-pentadecane
56	219	tripropylene glycol methyl ether
57	225	diethyl phthalate
57A	227	$C_{14}H_{28}O$ isomer
58	227	2,2,4-trimethylpenta-1,3-diol di-isobutyrate (BKG)
59	228	n-hexadecane

[a] See Table 27 for sampling protocol and Fig. 12 (L6) for sampling location.

Table B5. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH, LOUISIANA[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
3	45	chloromethane
4	46	vinyl chloride
4A	46	*n*-butane + butene isomer
4B	48	C_5H_{10} isomer
4C	49	chloroethane
5	49	isopentane
5B	50	C_5H_{10} isomer
6	51	acetaldehyde
6A	51	*n*-pentane
7	52	vinylidene chloride
8	53	dichloromethane
8A	54	propanal + propenal
8B	54	CS_2 + C_5H_8 isomer
8C	55	dimethyl ether
8D	56	acetone + C_5H_8 isomer
9	57	2-methylpentane
9A	58	1,1-dichloroethane
10	59	3-methylpentane
10A	60	C_6H_{12} isomer
11	60	hexafluorobenzene (eS)
11A	61	*n*-hexane
12	63	chloroform
13	65	perfluorotoluene (eS)
13A	65	methylcyclopentane
14	67	1,2-dichloroethane
14A	67	1,1,1-trichloroethane
15	70	benzene
15A	71	carbon tetrachloride
16	72	2-methylhexane
16A	73	2,3-dimethylpentane
17	74	3-methylhexane
18	76	1,2-dichloropropane
18A	77	C_8H_{18} isomer
18B	78	trichloroethylene
18C	78	dichloropropene isomer
19	79	*n*-heptane
20	84	methylcyclohexane
21	85	C_8H_{18} isomer
21A	86	C_8H_{18} isomer
21B	87	1,3-dichloropropane (tent.)
21C	87	C_8H_{16} isomer
22	89	C_8H_{18} isomer
22A	90	*n*-pentanal (tent.)
23	90	1,1,2-trichloroethane
24	92	toluene
24A	93	C_8H_{18} isomer
25	94	C_8H_{18} isomer
25A	95	C_8H_{16} isomer
25B	96	C_9H_{20} isomer
25C	98	C_8H_{16} isomer
25D	98	$C_6H_{12}O$ isomer
26	100	*n*-octane
27	101	tetrachloroethylene
27A	106	C_9H_{20} isomer
27B	107	C_8H_{16} isomer
27C	108	C_9H_{20} isomer
27D	108	C_9H_{18} isomer
27E	111	C_9H_{18} isomer
28	112	ethylbenzene
28A	113	C_9H_{20} + trichloropropene isomers
29	113	*p*-xylene
30	114	C_9H_{20} isomer
30A	117	C_9H_{18} isomer
31	118	*o*-xylene
31A	118	styrene
31B	119	1,1,2,2-tetrachloroethane
32	120	*n*-nonane
32A	122	C_9H_{18} isomer
33	124	isopropylbenzene + trichloropropene isomer (tent.)
33A	125	$C_{10}H_{20}$ isomer
33B	125	$C_{10}H_{22}$ isomer
33C	126	C_9H_{18} isomer
34	127	$C_{10}H_{22}$ isomer
34A	128	$C_{10}H_{22}$ isomer
34B	129	$C_{10}H_{20}$ isomer
34C	130	*n*-propylbenzene
34D	131	*m*-ethyltoluene
34E	132	tetrachloropropane isomer
35	133	$C_{11}H_{24}$ isomer
35A	133	pentachloroethane + 1,3,5-trimethylbenzene
35B	134	$C_{10}H_{22}$ isomer
36	135	*o*-ethyltoluene
36A	136	$C_{11}H_{24}$ + $C_{10}H_{18}$ isomers
36B	134	$C_{10}H_{20}$ isomer
37	137	benzaldehyde + 1,2,4-trimethylbenzene
38	139	*n*-decane
38A	140	$C_{10}H_{20}$ isomer

(continued)

Table B5 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
38B	141	dichlorobenzene isomer (tent.)
38C	142	$C_{11}H_{24}$ isomer
38D	142	C_4-alkyl benzene isomer
39	143	1,2,3-trimethylbenzene
39A	143	$C_{11}H_{24}$ isomer
39B	144	phenol (tent.)
39C	144	$C_{11}H_{24}$ isomer
39D	145	$C_{11}H_{22}$ isomer
40	146	$C_{10}H_{20}$ isomer
41	147	bis-(2-chloroisopropyl)ether
41A	148	C_5-alkyl benzene isomer
41B	149	C_4-alkyl benzene isomer
42	150	$C_{11}H_{24}$ isomer
43	152	hexachloroethane
43A	153	$C_{10}H_{12}$ isomer
43B	154	C_4-alkyl benzene isomer
44	155	acetophenone
44A	156	tetrachlorobutadiene isomer
45	157	n-undecane
45A	159	$C_{12}H_{26}$ isomer
46	160	C_4-alkyl benzene isomer
47	162	$C_{13}H_{28}$ isomer
48	163	$C_{11}H_{22}$ isomer
48A	164	C_5-alkyl benzene isomer
48B	165	$C_{10}H_{12}$ isomer
49	166	$C_{12}H_{26}$ + C_5-alkyl benzene isomers
49A	167	$C_{12}H_{24}$ isomer
49B	168	pentachlorobutadiene (tent.)
49C	169	$C_{12}H_{26}$ isomer
50	172	naphthalene
50A	172	$C_{10}H_{20}O$ isomer (tent.)
51	173	n-dodecane
52	176	1,3-hexachlorobutadiene
52A	188	$C_{13}H_{28}$ isomer
53	201	unknown
54A	214	$C_{15}H_{30}$ isomer
55	216	n-pentadecane
56	225	diethyl phthalate
57	228	n-hexadecane

[a] See Table 27 for sampling protocol and Fig. 12 (L7) for sampling location.

Table B6. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH, LOUISIANA[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2A	47	chloromethane
3	48	vinyl chloride (tent.) + 1-butene + *n*-butane
4	53	isopentane
4B	55	C_5H_{10} isomer
5	55	*n*-pentane
5A	56	C_5H_{10} isomer
6	57	acetaldehyde
6A	58	dichloromethane
6B	60	propanal
6C	61	propenal
6D	61	C_5H_{10} isomer
7	62	2-methylpentane
7A	63	dimethyl ether
7B	64	3-methylpentane
7C	65	acetone
8	66	hexafluorobenzene (eS)
8A	67	*n*-hexane
9	69	chloroform
10	71	perfluorotoluene (eS)
10A	74	1,1,1-trichloroethane
10B	74	*n*-butanal
10C	75	1,2-dichloroethane
11	76	benzene + carbon tetrachloride
12	78	2-methylhexane
13	80	3-methylhexane
13A	81	C_7H_{14} isomer
13B	82	C_8H_{18} isomer
13C	84	trichloroethylene
14	85	*n*-heptane
14A	87	*n*-pentanal (tent.)
15	89	methylcyclohexane
16	91	C_8H_{18} isomer
16A	92	C_8H_{16} isomer
16B	95	C_8H_{18} isomer
17	97	toluene
17A	98	C_8H_{18} isomer
17B	99	C_8H_{18} isomer
17C	100	C_8H_{16} isomer
17D	101	$C_6H_{12}O$ isomer
17E	103	C_8H_{16} isomer
18	105	*n*-octane
18A	106	C_8H_{16} isomer
18B	106	tetrachloroethylene
18C	107	2-hexanone
18D	110	C_9H_{20} isomer
18E	111	C_2-alkyl cyclohexane isomer
19	112	C_9H_{20} isomer
19A	113	C_9H_{18} isomer
19B	114	chlorobenzene
19C	115	C_9H_{18} isomer
20	116	ethylbenzene
21	117	*p*-xylene
21A	119	C_9H_{20} isomer
21B	120	phenylacetylene
22	122	*o*-xylene
22A	123	C_9H_{18} isomer + styrene (tent.)
23	124	*n*-nonane
23A	126	C_9H_{18} isomer
24	128	isopropylbenzene
24A	130	C_3-alkyl cyclohexane isomer
25	131	$C_{10}H_{22}$ isomer
25A	134	*n*-propylbenzene
25B	134	$C_{10}H_{22}$ isomer
25C	135	chlorotoluene isomer (tent.)
26	136	*p*-ethyltoluene
26A	137	$C_{10}H_{22}$ isomer
26B	138	$C_{10}H_{22}$ isomer
27	139	*o*-ethyltoluene
27A	140	$C_{10}H_{20}$ isomer
28	141	benzaldehyde
28A	142	C_3-alkyl benzene isomer
29	143	*n*-decane
29A	144	$C_{10}H_{20}$ isomer
29B	145	dichlorobenzene isomer (tent.)
30	147	$C_{11}H_{24}$ isomer + benzonitrile (tent.)
30A	148	phenol
31	149	$C_{10}H_{20}$ isomer
31A	150	$C_{11}H_{24}$ isomer
31B	151	C_4-alkyl benzene isomer
31C	152	$C_{11}H_{22}$ isomer
32	154	$C_{12}H_{26}$ isomer
32A	155	$C_{11}H_{22}$ isomer
32B	155	$C_{12}H_{26}$ isomer
33	158	acetophenone
34	160	*n*-undecane
34A	163	C_4-alkyl benzene isomer
34B	164	cresol isomer
34C	168	ethylphenol isomer
35	170	dimethylphenol isomer

(continued)

Table B6 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
36	174	naphthalene
36A	175	$C_{12}H_{24}$ isomer
36B	175	*n*-decanal
37	176	*n*-dodecane
37A	177	C_2-alkyl phenol isomer
37B	179	$C_{13}H_{28}$ isomer
38	184	aliphatic alcohol isomer (tent.)
39	191	*n*-tridecane
	192	β-methylnaphthalene
41	201	butyl butyrate
42	204	biphenyl (tent.)
43	205	*n*-tetradecane
44	214	$C_{15}H_{32}$ isomer
45	217	tridecanone isomer
45A	217	$C_{15}H_{30}$ isomer
46	218	*n*-pentadecane
47	230	2,2,4-trimethylpenta-1,3-diol di-isobutyrate
47A	231	*n*-hexadecane

[a] See Table 27 for sampling protocol and Fig. 11 (L8) for sampling location.

Table B7. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH, LOUISIANA[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
1B	45	chloromethane (tent.)
2	46	1-butene
2A	46	n-butane
2B	47	2-butene
3	49	isopentane
4	50	acetaldehyde
4A	51	n-pentane
4B	51	furan
4C	52	C_5H_{10} isomer
4D	53	dichloromethane
5	53	propanal + propenal + C_6H_{14} isomer
5A	54	dimethyl ether
5B	55	acetone
6	57	2-methylpentane
7	58	3-methylpentane
7A	59	C_4H_8O isomer
7B	59	n-butanal + C_6H_{12} isomer
8	60	hexafluorobenzene (e[illegible])
8A	61	n-hexane + methylfuran isomer
9	62	chloroform
10	64	perfluorotoluene (e[illegible])
11	67	1,1,1-trichloroethane
12	69	benzene
12A	70	carbon tetrachloride
12B	71	cyclohexane (tent.)
13	71	C_7H_{16} isomer
14	73	C_7H_{16} isomer
14A	75	C_7H_{14} isomer
15	76	C_8H_{18} isomer
16	78	n-heptane
16A	79	trichloroethylene
16B	82	C_8H_{18} isomer (tent.)
17	83	methylcyclohexane
17A	84	$C_6H_{12}O$ isomer (tent.)
18	85	C_8H_{18} isomer
18A	88	C_8H_{18} isomer (tent.)
19	91	toluene
19A	92	C_8H_{18} isomer
20	93	C_8H_{18} isomer
20A	94	C_8H_{16} isomer
20B	95	C_9H_{20} isomer
20C	97	C_8H_{16} isomer
21	99	n-octane
21A	100	tetrachloroethylene
21B	105	C_9H_{20} isomer
21C	106	C_8H_{16} isomer
21D	107	C_9H_{20} isomer
21E	107	C_9H_{18} isomer
21F	108	$C_7H_{14}O$ isomer
21G	109	chlorobenzene
21H	109	C_9H_{18} isomer
22	111	ethylbenzene
23	113	p-xylene
23A	114	C_9H_{20} isomer
23B	115	phenylacetylene (tent.)
24	117	o-xylene + C_9H_{18} isomer
25	119	n-nonane
25A	120	$C_{10}H_{22}$ isomer
25B	121	C_9H_{18} isomer
26	123	isopropylbenzene
26A	124	$C_{10}H_{20}$ isomer
26B	126	C_3-alkyl cyclohexane isomer
27	126	$C_{10}H_{22}$ isomer
27A	127	$C_{10}H_{22}$ isomer
27B	130	n-propylbenzene
27C	130	$C_{10}H_{22}$ isomer
27D	131	p-ethyltoluene
27E	132	$C_{10}H_{20}$ isomer
28	132	$C_{10}H_{22}$ isomer
29	133	$C_{10}H_{22}$ isomer
29A	134	C_3-alkyl benzene isomer
30	136	benzaldehyde + $C_{10}H_{20}$ isomer
30A	137	C_3-alkyl benzene isomer
31	139	n-decane
31A	139	n-octanal
31B	141	C_3-alkyl benzene isomer
31C	142	phenol
31D	143	$C_{11}H_{24}$ isomer
32	144	$C_{10}H_{20}$ isomer
32A	145	$C_{11}H_{24}$ isomer
32B	146	C_4-alkyl benzene isomer
32C	146	C_4-alkyl benzene isomer
32D	147	C_4-alkyl benzene + $C_{11}H_{22}$ isomers
	149	$C_{11}H_{24}$ isomer (tent.)
	151	C_4-alkyl benzene isomer
	152	C_4-alkyl benzene isomer
33	153	acetophenone
34	156	n-undecane
	161	$C_{11}H_{22}$ isomer

(continued)

Table B7 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
	171	naphthalene	37	225	diethyl phthalate
	172	$C_{10}H_{20}O$ isomer	38	227	aliphatic hydrocarbon isomer
35	173	*n*-dodecane	39	239	$C_{15}H_{30}O$ alkyl ketone isomer
	188	$C_{12}H_{26}$ + $C_{11}H_{14}$ isomers	40	240	*n*-hexadecane
	189	dimethylphenol isomer	41	240	unknown
36	198	butyl butyrate (tent.)			

---

[a] See Table 27 for sampling protocol and Fig. 11 (L9) for sampling location.

Table B8. VOLATILE ORGANICS IN AMBIENT AIR FROM IBERVILLE PARISH, LOUISIANA[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	43	CO_2
2A	46	C_4H_{10} isomer
2B	48	*n*-butane + C_4H_8 isomer
2C	52	isopentane
2D	54	C_5H_{10} isomer
2E	54	*n*-pentane
2F	55	furan
3	55	acetaldehyde
4	57	C_6H_{14} isomer
4A	59	propanal
4B	60	propenal
5	62	dimethyl ether
5A	63	C_6H_{14} isomer
5B	64	acetone
6	65	perfluorobenzene (eS)
6A	67	chloroform
7	70	perfluorotoluene (eS)
7A	72	*n*-butanal
7B	73	1,1,1-trichloroethane
7C	75	benzene + carbon tetrachloride
7D	77	C_6H_{16} isomer
7E	79	C_7H_{14} isomer
7F	81	C_7H_{14} isomer
7G	82	trichloroethylene
7H	83	*n*-heptane
7I	87	C_7H_{14} isomer
7J	89	C_8H_{18} isomer
7K	93	unsaturated hydrocarbon
7L	95	toluene
7M	96	C_8H_{18} isomer
7N	101	C_8H_{16} isomer
7O	103	*n*-octane
7P	104	tetrachloroethylene + hexanal
7Q	106	C_8H_{16} isomer
7R	110	unsaturated hydrocarbon
7S	114	ethylbenzene
8	116	*p*-xylene
8A	117	C_9H_{20} isomer
8B	120	*o*-xylene + styrene
9	122	*n*-nonane
9A	124	C_9H_{18} isomer
9B	124	*n*-heptanal
10	126	isopropylbenzene
10A	133	C_3-alkyl benzene isomer
11	134	$C_{10}H_{20}$ isomer + $C_{10}H_{22}$ isomer
12	136	C_3-alkyl benzene isomer
13	138	benzaldehyde
13A	139	C_3-alkyl benzene isomer
14	141	*n*-decane
14A	142	*n*-octanal
15	144	phenol + C_3-alkyl benzene
16	148	saturated hydrocarbon
16A	150	C_4-alkyl benzene isomer
17	151	unsaturated hydrocarbon
17A	153	$C_{10}H_{20}$ isomer
18	155	acetophenone
19	158	*n*-undecane
19A	161	C_4-alkyl benzene + unsaturated hydrocarbon isomers
20	167	dimethylphenol
21	171	unsaturated hydrocarbon + naphthalene
22	173	*n*-dodecane
23A	188	saturated hydrocarbon
24	197	alkyl isobutyrate
25	202	saturated hydrocarbon
26	218	saturated hydrocarbon
26A	225	diethyl phthalate
27	228	$C_{15}H_{32}$ isomer
28	230	*n*-hexadecane
29	240	unknown
30	240	unknown

[a] See Table 27 for sampling protocol and Fig. 11 (L11) for sampling location.

Table B9. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #17[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	40	CO_2
2	44	1-butene
3	47	isopentane
3A	48	C_5H_{10} isomer
4	49	n-pentane
5	50	acetaldehyde
6	52	dichloromethane
6A	52	CS_2
6B	53	propanal
6C	53	propenal
6D	55	C_5H_{10} isomer
7	56	2-methylpentane
7A	57	acetone (tent)
8	57	3-methylpentane
9	59	hexafluorobenzene (e[illegible])
10	60	n-hexane
11	61	chloroform
11A	64	C_7H_{16} isomer
12	65	methylcyclopentane
12A	65	perfluorotoluene (e[illegible])
13	67	1,1,1-trichloroethane
13A	68	1,2-dichloroethane
14	69	benzene
14A	70	carbon tetrachloride
15	70	cyclohexane
16	71	2-methylhexane
17	73	3-methylhexane
18	76	C_7H_{14} isomer
18A	77	trichloroethylene
19	78	n-heptane
19A	79	n-heptanal
19B	80	C_7H_{14} isomer
20	82	methylcyclohexane
20A	85	C_8H_{18} isomer
20B	86	C_8H_{16} isomer (tent)
21	91	toluene
22	92	C_8H_{18} isomer
22A	93	C_8H_{18} isomer
22B	94	ethylcyclohexane
22C	97	C_8H_{16} isomer
23	98	n-octane
23A	100	tetrachloroethylene
23B	105	ethylcyclohexane
23C	107	C_9H_{18} isomer
23D	110	ethylbenzene or xylene isomer
23E	116	$C_{10}H_{22}$ isomer (tent)
23F	117	C_9H_{18} isomer
24	119	n-nonane
24A	121	C_9H_{18} isomer
24B	122	$C_{10}H_{22}$ isomer (tent)
25	131	$C_{10}H_{22}$ isomer
26	133	n-decane
27	137	benzaldehyde
27A	147	phenol
28	154	acetophenone + n-nonanal
28A	162	cresol isomer
28B	165	C_2-alkyl phenol isomer
28C	168	C_2-alkyl phenol isomer
29	170	n-decanal
30	186	saturated hydrocarbon
31	196	butyl butyrate isomer (BKG)
32	199	n-tetradecane
33	208	$C_{15}H_{32}$ isomer (tent)
34	211	$C_{15}H_{30}$ isomer
35	213	n-pentadecane
38	225	n-hexadecane

[a] See Table 28 for sampling protocol.

Table B10. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #21[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	40	CO_2
1A	42	chloromethane (tent.) + propane
2	43	1-butene + n-butane
2A	44	2-butene
3	47	isopentane
3A	48	C_5H_{10} isomer
4	49	n-pentane + furan
4A	49	acetaldehyde
4B	50	C_5H_{10} isomer
5	51	dichloromethane
5A	51	carbon disulfide + propanal + propenal
5B	52	diethyl ether
5C	52	dimethyl ether
6	53	acetone
7	55	2-methylpentane
7A	56	isopropanol
8	57	3-methylpentane + ter-butanol
8A	58	chloroprene
9	58	hexafluorobenzene (eS)
9A	59	n-hexane
10	60	chloroform
10A	62	n-butanal
11	63	perfluorotoluene (eS)
11A	64	methylcyclopentane
11B	66	1,1,1-trichloroethane
11C	67	methyl ethyl ketone
12	68	benzene
12A	69	carbon tetrachloride (tent.)
12B	69	cyclohexane
12C	70	2-methylhexane
13	72	3-methylhexane
13A	73	C_7H_{14} isomer
13B	74	C_7H_{14} isomer
13C	75	trichloroethylene
14	76	n-heptane
15	81	methylcyclohexane
16	83	C_8H_{18} isomer
17	85	C_8H_{16} isomer (tent.)
18	88	toluene
18A	88	C_8H_{18} isomer
19	90	C_8H_{18} isomer + 2,3-dichlorobutane (tent.)
20	94	1,2-dichlorobutane (tent.)
21	96	n-octane
22	97	tetrachloroethylene
24	108	ethylbenzene
25	109	p-xylene
26	111	C_9H_{20} isomer
26A	113	styrene
27	114	o-xylene
28	116	n-nonane
28A	118	C_9H_{18} isomer
29	120	isopropylbenzene + $C_{10}H_{22}$ isomer
29A	122	$C_{10}H_{22}$ isomer
30	123	$C_{10}H_{22}$ isomer
31	125	n-propylbenzene
32	127	ethyltoluene isomer
32A	128	$C_{10}H_{22}$ isomer
33	128	$C_{11}H_{24}$ isomer
34	130	benzaldehyde + C_3-alkyl benzene isomer
34A	131	$C_{10}H_{22}$ isomer
35	133	C_3-alkyl benzene isomer
36	135	n-decane
36A	136	phenol
36B	138	C_4-alkyl benzene isomer
37	138	1,2,3-trimethylbenzene
38	139	$C_{11}H_{24}$ isomer
39	140	C_4-alkyl benzene isomer
39A	141	indan (tent.)
39B	141	C_4-alkyl cyclohexane isomer
40	142	$C_{11}H_{24}$ isomer
40A	143	C_4-alkyl benzene isomer
41	143	C_4-alkyl benzene isomer
42	144	C_4-alkyl benzene isomer
42A	146	$C_{11}H_{24}$ isomer
42B	146	C_4-alkyl benzene isomer
43	147	$C_{11}H_{24}$ isomer
43A	147	β-chlorostyrene (tent.)
43B	148	C_4-alkyl benzene isomer
44	148	acetophenone
45	150	cresol + C_4-alkyl benzene isomers
45A	151	$C_{11}H_{22}$ isomer
46	152	n-nonanal
47	153	n-undecane
47A	154	C_5-alkyl benzene isomer
48	155	$C_{11}H_{22}$ isomer
49	156	C_4-alkyl benzene isomer
50	157	$C_{12}H_{26}$ isomer

(continued)

Table B10 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
51	159	dimethylphenol + C_5-alkyl benzene isomers
51A	160	C_5-alkyl benzene isomer
51B	161	C_4-alkyl benzene isomer
52	162	$C_{12}H_{26}$ isomer
53	163	dimethylphenol isomer
54	164	$C_{13}H_{28}$ isomer
54A	166	naphthalene
54B	167	$C_{12}H_{24}$ isomer
55	167	*n*-decanal
56	168	*n*-dodecane
57	171	$C_{13}H_{28}$ isomer
58	173	chloroprene dimer
58A	180	$C_{14}H_{30}$ isomer (tent.)
58B	183	methylnaphthalene isomer
59	183	*n*-tridecane
61	189	chloro compound unknown
62	192	alkyl isobutyrate (tent.)
63	193	alkyl butyrate (tent.)
65	197	*n*-tetradecane
66	206	$C_{11}H_{16}O_2$ isomer (tent.)
67	211	$C_{15}H_{32}$ isomer
68	214	unknown
69	220	diethyl phthalate (BKG)
71	223	unknown
73	233	$C_{16}H_{32}$ isomer
74	235	*n*-hexadecane
77	240	unknown

[a] See Table 28 for sampling protocol.

Table B11. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #23[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	40	CO_2
2	43	propane (tent.)
2A	44	1-butene + n-butane
3	47	isopentane
3A	49	C_5H_{10} isomer
4	49	n-pentane
5	50	acetaldehyde
5A	51	C_5H_{10} isomer
5B	51	dichloromethane (tent.)
6	52	acetone
7	56	2-methylpentane
8	57	3-methylpentane
9	58	C_6H_{12} isomer
10	59	hexafluorobenzene (eB)
10A	59	n-hexane
10B	61	chloroform
11	63	perfluorotoluene (eF)
11A	64	methylcyclopentane
11B	64	C_7H_{16} isomer
12	66	1,1,1-trichloroethane
12A	67	1,2-dichloroethane
13	68	benzene
13A	69	carbon tetrachloride
14	70	cyclohexane
14A	71	2-methylhexane
15	72	3-methylhexane
16	74	C_7H_{14} isomer
16A	75	trichloroethylene
17	76	n-heptane
18	80	methylcyclohexane
18A	82	C_8H_{16} isomer
19	83	C_8H_{18} isomer
19A	85	C_8H_{16} isomer
19B	86	C_8H_{16} isomer
20	86	C_8H_{18} isomer
21	87	C_8H_{18} isomer
22	88	toluene
23	89	C_8H_{18} isomer
24	91	C_8H_{18} isomer
25	92	dimethylcyclohexane isomer
26	93	C_9H_{20} isomer (tent.)
27	95	C_8H_{16} isomer
28	96	n-octane
28A	97	C_8H_{16} isomer
29	98	tetrachloroethylene
29A	102	C_9H_{18} isomer
29B	102	C_9H_{20} isomer
30	103	C_8H_{16} isomer
30A	104	C_9H_{20} isomer
30B	104	C_9H_{18} isomer
30C	107	C_9H_{18} isomer
31	107	ethylbenzene
32	109	p-xylene + C_9H_{20} isomer
33	110	C_9H_{20} isomer
33A	111	C_9H_{18} isomer
34	112	styrene
35	113	o-xylene
36	116	n-nonane
36A	117	C_9H_{18} isomer
37	119	isopropylbenzene + $C_{10}H_{22}$ isomer
37A	121	$C_{10}H_{22}$ isomer
37B	122	C_9H_{18} isomer
38	122	$C_{10}H_{22}$ isomer
39	124	$C_{10}H_{20}$ isomer
39A	125	n-propylbenzene
39B	126	$C_{10}H_{22}$ isomer
40	127	ethyltoluene
41	128	$C_{10}H_{22}$ isomer
42	129	$C_{10}H_{22}$ isomer
42A	130	C_3-alkyl benzene isomer
43	131	$C_{10}H_{22}$ isomer
43A	132	$C_{10}H_{20}$ + C_4-alkyl benzene isomers
44	132	benzaldehyde + 1,2,4-trimethylbenzene
45	134	n-decane
45A	136	dichlorobenzene isomer (tent.)
45B	138	1,2,3-trimethylbenzene
46	139	$C_{11}H_{24}$ isomer
47	140	$C_{11}H_{24}$ isomer
48	141	C_4-alkyl cyclohexane isomer
49	142	C_4-alkyl benzene isomer
50	144	$C_{11}H_{22}$ + C_4-alkyl benzene isomers
51	145	$C_{11}H_{24}$ isomer
52	147	C_4-alkyl benzene isomer
52A	148	$C_{10}H_{12}$ isomer
53	149	acetophenone
54	151	$C_{11}H_{22}$ isomer
55	152	n-undecane
55A	154	cresol isomer

(continued)

Table B11 (cont'd)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
56	155	C_4-alkyl benzene isomer
56A	157	C_5-alkyl benzene isomer
57	159	dimethylphenol isomer
58	161	$C_{12}H_{26}$ isomer
58A	162	C_5-alkyl benzene isomer
59	162	$C_{12}H_{26}$ isomer (tent.)
60	163	$C_{12}H_{26}$ isomer
60A	164	ethylphenol isomer
60B	165	naphthalene
61	166	$C_{12}H_{24}$ isomer
62	167	n-decanal
63	167	n-dodecane
63A	169	$C_{12}H_{24}$ isomer
64A	181	$C_{13}H_{26}$ isomer
65	182	n-tridecane
65A	183	β-methylnaphthalene
67	192	$C_{14}H_{30}$ isomer (tent.)
68	195	$C_{14}H_{28}$ isomer
69	196	n-tetradecane
69A	200	C_2-alkyl naphthalene isomer
70	205	$C_{15}H_{32}$ isomer
71	210	n-pentadecane
72	213	unknown
73	219	diethyl phthalate (BKG)
76	233	2-tetradecanone
77	234	n-hexadecane
79	240	unknown
80	240	dialkyl phthalate isomer (BKG)
80A	240	dialkyl phthalate isomer (BKG)

[a] See Table 28 for sampling protocol.

Table B12. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #26[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	41	CO_2
1A	43	n-propane (tent)
1B	44	C_4H_8 isomer
1C	44	n-butane
1D	45	butadiene + C_4H_8 isomers
2	47	isopentane
3	49	C_5H_{10} isomer
3A	49	n-pentane + furan (tent)
4	50	acetaldehyde
4A	50	C_5H_{10} isomer
5A	51	dichloromethane
5B	52	propanal
5C	52	propenal
5D	53	dimethyl ether
5E	54	acetone + C_6H_{12} isomer
6	55	2-methylpentane
7	56	3-methylpentane
7A	57	C_6H_{12} + alcohol (tent) isomers
8	58	hexafluorobenzene (e[illegible])
9	59	n-hexane
10	60	chloroform
10A	61	pentanol isomer (tent)
11	62	perfluorotoluene (e[illegible])
11A	63	methylcyclopentane
11B	64	n-butanal
12	65	1,2-dichloroethane
13	67	benzene
13A	68	carbon tetrachloride (tent)
13B	68	cyclohexane
14	69	2-methylhexane
15	71	3-methylbenzene
15A	73	C_7H_{14} isomer
16	73	C_8H_{18} isomer
17	75	n-heptane
17A	78	C_7H_{14} isomer
18	80	methylcyclohexane
18A	81	C_8H_{16} isomer
19	82	C_8H_{18} isomer
19A	85	C_8H_{16} isomer
20	86	C_8H_{18} isomer
20A	86	C_9H_{20} isomer
20B	87	C_8H_{16} isomer
21	87	toluene
22	88	C_8H_{18} isomer
23	90	C_8H_{18} isomer
24	91	C_8H_{16} isomer
25	92	C_9H_{20} isomer
25A	93	hexanone isomer
26	94	cyclopentanone (tent)
26A	95	C_8H_{16} isomer
27	96	n-octane
28	97	tetrachloroethylene
28A	99	C_9H_{18} isomer (tent)
28B	100	saturated hydrocarbon
29	102	4-vinyl-1-cyclohexene
29A	103	C_8H_{16} isomer
29B	104	C_9H_{16} isomer
29C	106	C_9H_{18} isomer
30	108	ethylbenzene
30A	108	C_9H_{20} isomer
31	109	xylene + C_9H_{20} isomers
32	111	C_9H_{20} isomer
33	114	styrene or cyclooctatetraene + o-xylene
34	116	n-nonane
34A	118	C_9H_{18} isomer
35	120	isopropylbenzene
35A	123	C_3-alkyl cyclohexane isomer
36	124	$C_{10}H_{22}$ isomer
37A	126	$C_{10}H_{20}$ isomer
37B	126	n-propylbenzene
38	128	ethyltoluene isomer
39	129	$C_{10}H_{22}$ isomer
39A	130	1,3,5-trimethylbenzene (tent)
40	130	$C_{10}H_{22}$ isomer
40A	131	o-ethyltoluene
40B	132	benzaldehyde
40C	133	$C_{10}H_{20}$ isomer
41	134	1,2,4-trimethylbenzene
42	136	n-decane
42A	139	C_4-alkyl benzene isomer
42B	139	1,2,3-trimethylbenzene
43	140	$C_{11}H_{24}$ isomer + phenol (tent)
44	142	$C_{10}H_{20}$ isomer
45	143	$C_{11}H_{24}$ isomer
45A	144	C_4-alkyl benzene + $C_{11}H_{24}$ (tent) isomers
45B	145	C_4-alkyl benzene + n-butylbenzene
45C	146	$C_{11}H_{22}$ isomer (tent)
46	147	$C_{11}H_{24}$ isomer
47	149	C_4-alkyl benzene isomer

(continued)

Table B12 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
47A	149	$C_{11}H_{22}$ isomer
48	150	acetophenone
49	153	$C_{11}H_{22}$ isomer
50	153	*n*-undecane
51	156	C_4-alkyl benzene isomer
51A	157	cresol isomer (tent.)
51B	158	$C_{12}H_{26}$ isomer
51C	159	C_5-alkyl benzene isomer
51D	160	$C_{12}H_{24}$ isomer
51E	161	methylindan isomer (tent.)
52	162	dimethylphenol isomer
52A	164	C_5-alkyl benzene isomer
52B	166	C_2-alkyl phenol isomer
53	167	naphthalene
53A	169	$C_{12}H_{24}$ isomer
54	170	*n*-dodecane
55	172	1,3-hexachlorobutadiene
56	178	unknown
56A	181	$C_{14}H_{30}$ isomer
57	184	*n*-tridecane
57A	185	methylnaphthalene
58	187	$C_8H_{18}O$ isomer *or* unknown
59	194	C_4-alkyl butyrate isomer
60	198	*n*-tetradecane
60A	202	C_2-alkyl naphthalene isomer
61	207	$C_{15}H_{32}$ isomer
61A	210	$C_{15}H_{30}$ isomer
62	211	*n*-pentadecane
63	214	alcohol *or* unknown
65A	225	$C_{14}H_{22}O$ alkyl phenol isomer (tent.)
66A	231	saturated hydrocarbon
67	235	$C_{17}H_{36}$ isomer
68	236	*n*-hexadecane *or* sat. hydrocarbon
70	240	unknown

[a] See Table 28 for sampling protocol.

Table B13. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #27[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	41	CO_2
1A	43	*n*-propane
1B	43	butene isomer
2	44	*n*-butane
3	47	isopentane
3A	48	C_5H_{10} isomer
4	49	*n*-pentane
4A	50	C_5H_{10} isomer
5	50	acetaldehyde
5A	51	C_5H_{10} isomer
6A	52	dichloromethane + C_6H_{14} isomer (tent)
6B	52	propanal
6C	53	propenal (tent)
6D	55	C_6H_{12} isomer
7	55	2-methylpentane
7A	56	methyl ethyl ketone
8	57	3-methylpentane
9	59	hexafluorobenzene (eS)
9A	59	*n*-hexane
10	61	chloroform
10A	63	alcohol (tent)
11	63	perfluorotoluene (eS)
11A	64	methylcyclopentane
11B	65	*n*-butanal
11C	66	1,1,1-trichloroethane
12	66	1,2-dichloroethane
13	68	benzene
13A	69	carbon tetrachloride
13B	69	cyclohexane
14	70	2-methylhexane
14A	71	2,3-dimethylpentane
15	72	3-methylhexane
15A	73	$C_5H_{10}O$ isomer (tent)
15B	73	C_7H_{14} isomer
16	74	C_8H_{18} isomer
17	76	*n*-heptane
18	81	methylcyclohexane
18A	82	*n*-pentanal (tent)
18B	82	C_8H_{16} isomer
19	83	C_8H_{18} isomer
20	86	C_8H_{18} isomer
20A	87	C_8H_{18} isomer
21	88	toluene
22	89	C_8H_{18} isomer
23	91	C_8H_{18} isomer
23A	92	C_8H_{16} isomer
23B	93	C_9H_{20} isomer
23C	94	C_8H_{16} isomer
24	96	*n*-octane
24A	97	C_8H_{16} isomer
24B	98	tetrachloroethylene
24C	100	C_9H_{20} isomer
24D	101	acetic acid (tent)
24E	102	C_9H_{20} isomer
24F	103	ethylcyclohexane
24G	107	C_9H_{18} isomer (tent)
25	108	ethylbenzene
26	109	xylene isomer
26A	110	C_9H_{20} isomer
27	111	C_9H_{20} isomer
27A	114	styrene
28	114	*o*-xylene
28A	115	C_9H_{18} isomer
29	116	*n*-nonane
29A	118	C_9H_{18} isomer
29B	119	$C_{10}H_{22}$ isomer
30	120	isopropylbenzene
31	123	$C_{10}H_{22}$ isomer
31A	125	*n*-propylbenzene
31B	126	$C_{10}H_{22}$ isomer
32	127	ethyltoluene isomer
33	128	$C_{10}H_{22}$ isomer
33A	129	1,3,5-trimethylbenzene (tent)
33B	130	*o*-ethyltoluene
34	131	$C_{10}H_{22}$ isomer
34A	132	$C_{10}H_{20}$ isomer
35	133	1,2,4-trimethylbenzene
35A	134	benzaldehyde
36	135	*n*-decane
36A	137	C_4-alkyl benzene
36B	138	1,2,3-trimethylbenzene
36C	139	$C_{11}H_{24}$
36D	140	indan
36E	141	$C_{10}H_{20}$
37	142	$C_{11}H_{24}$
37A	143	C_4-alkyl benzene
37B	144	*n*-butylbenzene + C_4-alkyl benzene isomer
38	146	$C_{11}H_{24}$
38A	148	C_4-alkyl benzene
38B	150	acetophenone

(continued)

Table B13 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
38C	150	$C_{11}H_{22}$
39	151	n-nonanal
40	152	n-undecane
40A	153	cresol
40B	154	C_4-alkyl benzene
40C	157	cresol
41	160	dimethylphenol
41A	162	C_5-alkyl benzene
42	165	naphthalene
42A	166	$C_{12}H_{24}$
43	167	n-decanal
43A	167	n-dodecane
44	175	unknown
44A	182	$C_{13}H_{26}$
45	183	n-undecanal
45A	183	n-tridecane + methylnaphthalene isomer
46	186	unknown
49	197	n-tetradecane
50	205	biphenylene
51A	209	$C_{15}H_{30}$
52	210	n-pentadecane
53	213	unknown
54	219	diethyl phthalate (BKG)
55A	222	n-hexadecane (tent)
56	233	$C_{17}H_{36}$
57	234	n-heptadecane

[a] See Table 28 for sampling protocol.

Table B14. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #28[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	41	CO_2
1A	44	propane
1B	45	*n*-butane
2	47	isopentane
3	49	*n*-pentane
3A	50	acetaldehyde
3B	51	C_5H_{10} isomer
4A	52	dichloromethane
4B	52	C_5H_6 isomer (tent)
4C	53	propenal (tent) + propanal
4D	54	C_6H_{12} isomer
5	56	2-methylpentane
5A	56	acetone
6	57	3-methylpentane
6A	58	C_6H_{12} isomer
7	59	hexafluorobenzene (eI)
7A	60	*n*-hexane
7B	61	C_6H_{12} isomer
7C	61	chloroform
8	62	di-isopropyl ether
9	64	perfluorotoluene (eI)
9A	64	methylcyclopentane
10	66	1,2-dichloroethane
10A	68	C_7H_{14} isomer
11	69	benzene
11A	69	carbon tetrachloride
11B	70	cyclohexane
12	71	2-methylhexane
12A	71	2,3-dimethylpentane
13	73	3-methylhexane
13A	74	C_7H_{14} isomer
13B	75	C_7H_{14} isomer
14	75	C_8H_{18} isomer
15	77	*n*-heptane
16	82	methylcyclohexane
16A	83	C_8H_{16} isomer
17	84	C_8H_{18} isomer
17A	85	C_8H_{16} isomer
18	87	C_8H_{18} isomer
19	89	toluene
20	90	C_8H_{18} isomer
21	92	C_8H_{18} isomer
21A	93	C_8H_{16} isomer
21B	94	C_8H_{18} isomer
21C	96	C_8H_{16} isomer
22	97	*n*-octane
22A	98	C_8H_{16} isomer
23	99	tetrachloroethylene
24	102	C_9H_{20} isomer
25	104	4-vinyl-1-cyclohexene
25A	104	ethylcyclohexane
25B	106	C_9H_{18} isomer
26	109	ethylbenzene
27	111	xylene isomer
28	112	C_9H_{20} isomer
29	114	styrene
30	115	*o*-xylene
30A	116	C_9H_{18}isomer
31	118	*n*-nonane
31A	119	C_9H_{18} isomer
32	121	isopropylbenzene
32A	124	C_3-alkyl cyclohexane isomer
33	124	$C_{10}H_{22}$ isomer
33A	127	*n*-propylbenzene
34	128	ethyltoluene isomer
35	130	$C_{10}H_{22}$ isomer + 1,3,5-trimethylbenzene
35A	132	*o*-ethyltoluene
35B	133	1-methyl-4-isopropylcyclohexane
35C	134	benzaldehyde
36	134	1,2,4-trimethylbenzene
36A	135	$C_{10}H_{20}$ isomer (tent)
37	136	*n*-decane
37A	139	C_4-alkyl benzene isomer
37B	140	1,2,3-trimethylbenzene
38	141	$C_{11}H_{24}$ isomer
38A	142	phenol
38B	142	indan (tent)
38C	143	$C_{11}H_{24}$ isomer
39	144	C_4-alkyl benzene isomer
40	145	C_4-alkyl benzene isomer + *n*-butylbenzene
41	147	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
42	149	C_4-alkyl benzene isomer
42A	150	$C_{11}H_{22}$ isomer
43	150	C_4-alkyl benzene isomer
43A	151	acetophenone
44	153	*n*-nonanal
45	153	*n*-undecane
45A	154	C_4-alkyl benzene isomer

(continued)

Table B14 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
45B	154	cresol isomer
45C	155	$C_{11}H_{22}$ isomer
46	156	C_4-alkyl benzene isomer
47	161	dimethylphenol isomer
48	165	C_2-alkyl phenol isomer
49	167	naphthalene
50	168	C_2-alkyl phenol + $C_{12}H_{24}$ isomers
50A	169	n-decanal
51	169	n-dodecane
52	177	alkylhydroxy butyrate isomer or unknown
52A	178	C_2-alkyl phenol isomer
52B	183	$C_{13}H_{26}$ isomer
53	184	n-tridecane
53A	184	β-methylnaphthalene
54	187	$C_6H_{14}O$ alcohol isomer (tent.)
57	198	n-tetradecane
57A	205	biphenylene
58	206	sat. hydrocarbon (tent.)
59	211	n-pentadecane
62A	224	n-hexadecane
63	224	C_9-alkyl phenol isomer (tent.)
64	230	unknown
65	234	$C_{15}H_{30}O$ isomer (tent.)
66	235	n-heptadecane
67	240	unknown
68	240	saturated hydrocarbon

[a] See Table 28 for sampling protocol.

Table B15. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #30[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	41	CO_2
1A	45	n-butane + butene isomer
2	49	isopentane
2A	51	C_5H_{10} isomer
3	51	n-pentane
4	52	acetaldehyde
4A	53	C_5H_{10} isomer
5A	55	dichloromethane (tent)
5B	57	C_6H_{12} isomer
6	58	2-methylpentane
7	60	3-methylpentane
7A	61	C_6H_{12} isomer
8	62	hexafluorobenzene (eS)
9	63	n-hexane
9A	65	chloroform
9B	66	C_4H_8O isomer (tent)
10	67	perfluorotoluene (eS)
10A	67	methylcyclopentane
10B	70	1,1,1-trichloroethane
10C	71	n-butanal
10D	71	1,2-dichloroethane
11	72	benzene
11A	72	carbon tetrachloride (tent)
12	73	cyclohexane
13	74	2-methylhexane
13A	74	2,3-dimethylpentane (tent)
14	75	3-methylhexane
14A	77	C_7H_{14} isomer
15	78	C_7H_{14} isomer
15A	78	C_8H_{18} isomer
16	79	n-heptane
16A	82	C_7H_{14} isomer
17	84	methylcyclohexane
18	86	C_8H_{18} isomer
18A	87	$C_6H_{12}O$ isomer
19	87	C_8H_{16} isomer
19A	88	C_8H_{16} isomer
20	89	C_8H_{18} isomer
20A	90	C_8H_{18} isomer
21	91	toluene
22	92	C_8H_{18} isomer
23	94	C_8H_{18} isomer
24	95	dimethylcyclohexane isomer
25	96	C_9H_{20} isomer
26	98	C_8H_{16} isomer
27	100	n-octane
27A	101	C_8H_{16} isomer
27B	102	C_9H_{20} isomer
28	103	C_9H_{20} isomer
29	105	C_9H_{20} isomer
29A	105	ethylcyclohexane
30	106	C_9H_{18} isomer
30A	109	C_9H_{18} isomer
31	110	ethylbenzene
32	112	C_9H_{20} + xylene isomers
33	113	C_9H_{20} isomer
33A	114	C_9H_{18} isomer
33B	115	C_9H_{18} isomer
34	116	o-xylene
34A	116	C_9H_{18} isomer + styrene
35	118	n-nonane
35A	120	C_9H_{18} isomer
35B	121	$C_{10}H_{22}$ isomer
36	122	isopropylbenzene
36A	123	$C_{10}H_{22}$ isomer
36B	124	propylcyclohexane
37	125	$C_{10}H_{22}$ isomer
38	126	$C_{10}H_{22}$ isomer (tent)
38A	128	n-propylbenzene + $C_{10}H_{20}$ isomer
39	129	ethyltoluene isomer
40	130	$C_{10}H_{22}$ isomer
40A	130	C_3-alkyl benzene isomer
41	131	$C_{10}H_{22}$ isomer
42	132	ethyltoluene isomer
42A	134	$C_{10}H_{20}$ isomer
43	135	1,2,4-trimethylbenzene
43A	136	benzaldehyde
44	136	n-decane
45	140	1,2,3-trimethylbenzene
45A	141	$C_{11}H_{24}$ isomer
46	143	dichlorobenzene (tent) + C_4-alkyl cyclohexane isomers
47	144	$C_{11}H_{24}$ isomer
47A	145	C_4-alkyl benzene isomer
47B	146	C_4-alkyl benzene isomer
48	147	$C_{11}H_{24}$ isomer
49	149	$C_{11}H_{24}$ isomer
49A	149	C_4-alkyl benzene isomer
49B	150	$C_{11}H_{24}$ isomer
50	151	$C_{10}H_{12}$ isomer
50A	152	acetophenone

(continued)

Table B15 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
51	153	*n*-undecane
51A	155	C_4-alkyl benzene isomer
52	156	$C_{12}H_{26}$ isomer
52A	160	C_5-alkyl benzene isomer
53	162	C_2-alkyl phenol + C_4-alkyl benzene isomers
53A	162	C_5-alkyl benzene isomer
53B	165	C_2-alkyl phenol isomer
54	167	naphthalene + $C_{12}H_{24}$ isomer
55	169	*n*-dodecane
56	171	$C_{13}H_{28}$ isomer
56A	173	$C_{12}H_{24}$ isomer
56B	176	C_6-alkyl cyclohexane isomer
56C	183	$C_{13}H_{26}$ isomer
57	184	*n*-tridecane
57A	185	methylnaphthalene isomer
57B	186	methylnaphthalene + C_7-alkyl cyclohexane isomers
57C	192	$C_{14}H_{30}$ isomer (tent.)
58	194	alkyl butyrate (BKG)
59	198	*n*-tetradecane
59A	199	$C_{14}H_{28}$ isomer
59B	202	C_2-alkyl naphthalene isomer
59C	205	$C_{14}H_{28}$ isomer (tent.)
60	207	$C_{15}H_{32}$ isomer
61	210	unsat. hydrocarbon (tent.)
62	211	*n*-pentadecane
65	223	*n*-hexadecane
67	234	$C_{17}H_{36}$ isomer (tent.)
68	235	*n*-heptadecane
69	237	unsaturated hydrocarbon

[a] See Table 28 for sampling protocol.

Table B16. VOLATILE ORGANIC VAPORS IN AMBIENT AIR OF BATON ROUGE, LA AT LOCATION #26[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	41	CO_2
1A	44	butene isomer
2	45	1,3-butadiene
2A	46	C_4H_4 isomer (tent)
2B	47	1,2-butadiene (tent)
3	48	isopentane
3A	49	C_5H_{10} isomer
4	50	_n_-pentane
4A	50	C_5H_8 isomer
5	51	C_5H_{10} isomer + acetaldehyde
6A	52	dichloromethane + C_5H_8 isomer
7	53	$C_4H_{10}O$ isomer
8	54	cyclopentene
8A	55	_t_-butanol + C_6H_{12} isomer
9	56	2-methylpentane
11	59	C_6H_{12} isomer
12	59	hexafluorobenzene (eS)
13	60	_n_-hexane
14	60	di-isopropyl ether
15	64	perfluorotoluene (eS)
15A	64	methylcyclopentane
15B	65	$C_6H_{14}O$ isomer
16	66	1,2-dichloroethane
17	69	benzene
17A	69	carbon tetrachloride
17B	70	cyclohexane
18	71	2-methylhexane
19	73	3-methylhexane
19A	74	C_7H_{14} isomer
20	75	C_8H_{18} isomer
20A	76	trichloroethylene
21	77	_n_-heptane
22	79	C_8H_{16} isomer
23	82	methylcyclohexane
23A	83	C_8H_{16} isomer
24	84	C_8H_{18} isomer
24A	86	C_8H_{16} isomer
25	87	C_8H_{18} isomer
25A	89	1,1,2-trichloroethane
26	89	toluene
27	90	C_8H_{18} isomer
28	92	C_8H_{18} isomer
29	93	dimethylcyclohexane isomer
30	95	C_8H_{16} isomer
31	97	_n_-octane
32	98	tetrachloroethylene
33	101	C_9H_{20} isomer
34	103	4-vinyl-1-cyclohexene
34A	104	C_9H_{20} isomer (tent)
34B	105	1,1,1,2-tetrachloroethane
35	107	C_9H_{18} isomer
36	108	ethylbenzene
37	110	xylene isomer
37A	110	C_9H_{18} isomer
38	111	C_9H_{20} isomer
38A	112	C_9H_{18} isomer
38B	114	styrene _or_ cyclooctatetraene
39	114	_o_-xylene
40	116	_n_-nonane
41	119	C_9H_{12} isomer + isopropylbenzene
42	120	$C_{10}H_{22}$ isomer
43	123	$C_{10}H_{22}$ siomer
43A	125	_n_-propylbenzene
44	127	ethyltoluene isomer
45	128	1,3,5-trimethylbenzene + $C_{10}H_{22}$ isomer
45A	130	$C_{10}H_{22}$ isomer
46	131	_o_-ethyltoluene
46A	132	$C_{10}H_{22}$ isomer
46B	132	$C_{10}H_{20}$ isomer
47	133	1,2,4-trimethylbenzene
47A	134	methylstyrene _or_ C_9H_{10} isomer
48	135	_n_-decane
48A	136	benzaldehyde (tent)
48B	138	C_4-alkyl benzene isomer (tent)
49	139	1,2,3-trimethylbenzene
49A	141	indan _or_ C_9H_{10} isomer
49B	144	C_4-alkyl benzene isomer
50	145	_n_-butylbenzene + C_4-alkyl benzene isomer
50A	145	$C_{11}H_{22}$ isomer
50B	146	$C_{11}H_{24}$ isomer
51	147	C_4-alkyl benzene isomer
52	148	C_4-alkyl benzene isomer
53	150	C_4-alkyl benzene + $C_{11}H_{22}$ isomers

(continued)

Table B16 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
53A	151	acetophenone
54	152	*n*-nonanal
55	153	*n*-undecane
55A	154	cresol isomer (tent.)
55B	155	$C_{11}H_{22}$ isomer
56	156	C_4-alkyl benzene isomer
56A	157	cresol isomer
56B	159	C_5-alkyl benzene isomer
57	161	dimethylphenol isomer
57A	162	C_5-alkyl benzene isomer
57B	165	C_2-alkyl phenol isomer
58	166	naphthalene
59	168	*n*-decanal
59A	169	*n*-dodecane
60	171	1,3-hexachlorobutadiene
60A	174	unsaturated hydrocarbon
61	177	unknown
62	183	*n*-tridecane + β-methylnaphthalene
63	186	α-methylnaphthalene
66	197	*n*-tetradecane
66A	200	dimethylnaphthalene isomer
67	206	sat. hydrocarbon (tent.)
68	209	$C_{15}H_{30}$ isomer (tent.)
69	211	*n*-pentadecene
70	214	unknown
71	220	diethylphthalate (BKG)
73	223	*n*-hexadecane
74	234	$C_{15}H_{30}O$ isomer (tent.)
75	235	*n*-heptadecane
77	240	unknown

[a] See Table 28 for sampling protocol.

Part II

Linden and Deepwater, NJ

Table B17. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P1/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
1A	48	*n*-propane (tent.)
2A	52	*n*-butane
2B	53	butene isomer
3	54	acetaldehyde
3A	57	C_3H_8O isomer (tent.)
4	59	C_5H_{10} isomer
5	62	isopentane
6A	64	C_5H_{10} isomer
6B	64	furan
7	65	*n*-pentane
7A	66	propanal
7B	66	C_5H_{10} isomer
7C	68	C_5H_{10} isomer
7D	68	dichloromethane
8	69	acetone
10A	76	*t*-butanol
10B	77	C_4H_8O isomer (tent.)
11	78	2-methylpentane
11A	80	2-butenal or C_4H_6O isomer
12	81	3-methylpentane
12A	82	C_6H_{12} isomer + unknown
13	83	hexafluorobenzene (eI)
14	84	*n*-hexane
14A	85	C_6H_{12} isomer
15	86	chloroform
15A	87	C_6H_{12} isomer
15B	88	methyl ethyl ketone
16	90	perfluorotoluene (eI)
16A	90	C_7H_{16} isomer
17	91	C_7H_{16} isomer + methylcyclopentane
17A	93	C_7H_{16} isomer
18	94	1,1,1-trichloroethane
18A	96	C_6H_{10} isomer
18B	97	benzene
19	98	3,3-dimethylpentane
19A	99	carbon tetrachloride
19B	99	cyclohexane
20	100	2-methylhexane
21	101	2,3-dimethylpentane
22	102	3-methylhexane
22A	104	dimethylcyclopentane or C_7H_{14} isomer
23	105	dimethylcyclopentane or C_7H_{14} isomer
24	106	1-heptene + trichloroethylene
25	107	*n*-heptane
25A	108	C_7H_{14} isomer
25B	110	acetic acid (tent.)
26	113	C_8H_{18} isomer
27	114	methylcyclohexane
27A	115	C_8H_{18} isomer
28	116	C_8H_{18} isomer
28A	117	C_8H_{16} isomer
29	118	C_8H_{18} isomer (tent.)
30	120	C_8H_{16} isomer
30A	121	$C_6H_{12}O$ ketone isomer (tent.)
31	122	toluene
31A	123	C_8H_{18} isomer
32	124	C_8H_{18} isomer
33	127	C_8H_{16} isomer
33A	129	C_8H_{16} isomer
34	130	*n*-octane
34A	131	C_8H_{16} isomer
34B	131	C_8H_{14} isomer (tent.)
35	132	tetrachloroethylene
35A	133	C_8H_{16} isomer
37	136	C_9H_{20} isomer
38	137	C_9H_{20} isomer
38A	137	C_9H_{18} isomer
39	138	C_9H_{20} isomer
40	139	C_2-alkyl cyclohexane isomer
40A	139	chlorobenzene (tent.)
41	141	C_9H_{18} isomer
42	142	ethylbenzene
42A	143	C_9H_{18} isomer
42B	144	C_9H_{20} isomer
43	144	xylene isomer
44	145	C_9H_{20} isomer
44A	147	C_9H_{18} isomer
45	147	$C_{10}H_{22}$ isomer (tent.)
45A	148	C_9H_{18} isomer + styrene
46	149	*o*-xylene
46A	150	C_9H_{18} isomer
47	151	*n*-nonane
47A	153	$C_{10}H_{20}$ isomer
47B	154	C_9H_{18} isomer
48	155	$C_{10}H_{22}$ isomer
49	156	isopropylbenzene
49A	156	$C_{10}H_{22}$ isomer
49B	157	C_9H_{16} isomer

(continued)

Table B17 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
50	158	$C_{10}H_{22}$ isomer
51	159	propylcyclohexane or C_9H_{18} isomer
51A	160	$C_{10}H_{22}$ isomer
51B	160	$C_{10}H_{20}$ isomer
52	161	*n*-propylbenzene
52A	162	benzaldehyde + phenol
53	162	ethylbenzene isomer
53A	163	$C_{10}H_{22}$ isomer
54	164	1,3,5-trimethylbenzene
54A	164	$C_{11}H_{24}$ isomer (tent.)
54B	165	$C_{10}H_{20}$ isomer
55	166	*o*-ethylbenzene
56	168	$C_{10}H_{20}$ isomer
57	169	1,2,4-trimethylbenzene
58	169	*n*-decane
58A	171	$C_{10}H_{20}$ isomer
58B	172	C_4-alkyl benzene + dichlorobenzene (tent.) isomer
59	172	$C_{11}H_{24}$ isomer
60	173	C_4-alkyl benzene isomer
60A	174	$C_{11}H_{24}$ isomer
61	174	1,2,3-trimethylbenzene
61A	176	*o*-dichlorobenzene
62	177	indan
62A	177	C_4-alkyl cyclohexane isomer
62B	178	$C_{11}H_{22}$ isomer
63	179	C_4-alkyl benzene isomer
63A	179	*p*-propyltoluene
64	180	*n*-butylbenzene + diethylbenzene isomer
64A	180	$C_{11}H_{24}$ isomer
65	181	acetophenone
65A	182	C_4-alkyl benzene isomer
66	182	$C_{11}H_{24}$ isomer
67	184	dimethylethylbenzene isomer
68	185	*n*-nonanal
68A	186	methylindan + $C_{11}H_{22}$ isomers
69	187	*n*-undecane
70	188	C_5-alkyl benzene + $C_{11}H_{22}$ isomers
70A	189	C_4-alkyl benzene isomer
71	189	C_5-alkyl benzene isomer
71A	190	$C_{12}H_{24}$ isomer
71B	190	$C_{12}H_{26}$ isomer
72	191	tetramethylbenzene isomer
73	192	$C_{12}H_{24}$ isomer
73A	192	C_2-alkyl phenol isomer (tent.)
73B	193	$C_{11}H_{20}$ isomer (tent.)
74	193	C_5-alkyl benzene isomer
75	195	C_4H_7-benzene + C_5-alkyl cyclohexane isomers
76	196	$C_{12}H_{26}$ isomer
77	197	C_4H_7 benzene + C_4-alkyl benzene + C_5-alkyl benzene isomers
78	199	C_5-alkyl benzene isomer
79	200	C_5-alkyl benzene + $C_{12}H_{24}$ isomer
79A	201	C_6-alkyl benzene isomer
80	202	*n*-decanal
81	203	*n*-dodecane + naphthalene
81A	204	C_5-alkyl benzene isomer
81B	205	$C_{12}H_{24}$ isomer
82	206	$C_{13}H_{28}$ isomer
83	207	C_6-alkyl benzene isomer
83A	208	$C_{12}H_{22}$ isomer
84	210	$C_{13}H_{26}$ isomer (tent.)
85	211	$C_{12}H_{24}$ isomer
86	213	C_5H_9 benzene isomer
87	215	$C_{14}H_{30}$ isomer
87A	217	$C_{13}H_{26}$ isomer
88	218	*n*-tridecane
88A	219	$C_{13}H_{26}$ isomer
89	220	β-methylnaphthalene
89A	222	$C_{14}H_{28}$ isomer
90	223	α-methylnaphthalene
91	226	$C_{13}H_{26}$ isomer
92	229	$C_{14}H_{30}$ isomer
93	230	saturated hydrocarbon isomer (tent.)
93A	232	$C_{15}H_{30}$ isomer
94	233	*n*-tetradecane
94A	234	$C_{14}H_{28}$ isomer
94B	235	C_2-alkyl naphthalene isomer
94C	237	C_2-alkyl naphthalene isomer
95	239	$C_{15}H_{30}$ + dimethylnaphthalene isomers
96	240	$C_{16}H_{32}$ isomer
97	240	$C_{16}H_{34}$ isomer
98	240	$C_{15}H_{30}$ isomer
99	240	ketone (?)
99A	240	$C_{15}H_{30}$ isomer

(continued)

Table B17 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
100	240	n-pentadecane
103	240	n-hexadecane
104	240	$C_{15}H_{30}O$ isomer (tent.)
105	240	n-heptadecane
106	240	$C_{17}H_{34}$ isomer

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B18. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P1/L2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2A	50	chloromethane
2B	51	propane (tent.)
2C	52	C_4H_{10} isomer
2D	53	butene isomer
2E	54	*n*-butane
3	54	acetaldehyde
3A	56	bromomethane (tent.)
4	58	C_3H_8O isomer (tent.)
4A	59	C_5H_{12} isomer
5	61	isopentane
6A	65	acrolein
7	65	*n*-pentane
7A	66	*n*-propanal
7B	66	C_5H_8 isomer
7C	67	C_5H_{10} isomer
7D	68	2-thiapropane
7E	69	dichloromethane
7F	70	acetone
8A	74	C_3H_8O isomer
8B	79	*t*-butanol
9	80	2-methylhexane
9A	82	2-methylpropenal
10	83	3-methylhexane
11	85	hexafluorobenzene (eS)
12	86	*n*-hexane
13	87	chloroform
13A	88	methyl vinyl ketone (tent.) + C_6H_{12} isomer
13B	89	methyl ethyl ketone
14	91	perfluorotoluene (eS)
14A	92	C_7H_{16} isomer
15	93	C_7H_{16} isomer
16	95	trimethylbutane isomer
16A	95	1,1,1-trichloroethane
16B	98	C_6H_{10} isomer
16C	98	benzene
17	99	3,3-dimethylpentane
17A	100	carbon tetrachloride + cyclohexane
18	101	2-methylhexane
19	102	2,[illegible]-dimethylpentane
20	104	3-methylhexane
21	106	3-ethylpentane
22	107	C_7H_{14} isomer + trichloroethylene
23	109	*n*-heptane
23A	110	C_7H_{14} isomer
24	115	C_8H_{18} isomer
25	116	methylcyclohexane
26	118	C_8H_{18} isomer
26A	118	2,3-dithiabutane
27	120	C_8H_{16} isomer
28	122	C_8H_{16} + $C_6H_{12}O$ isomers
29	124	toluene
29A	125	C_8H_{18} isomer
30	126	C_8H_{18} isomer
31	129	C_8H_{16} isomer
31A	131	C_8H_{16} isomer
32	132	*n*-octane
33	134	tetrachloroethylene
34	138	unknown + C_9H_{20} isomer
35	140	C_9H_{20} isomer
36	141	chlorobenzene
36A	142	C_9H_{18} isomer
37	144	ethylbenzene
38	146	xylene isomer
39	147	C_9H_{20} isomer
39A	148	$C_{10}H_{22}$ isomer
40	149	styrene + C_9H_{18} isomer
40A	150	cyclohexanone
41	150	*o*-xylene
41A	151	C_9H_{18} isomer
42	152	*n*-nonane
43	153	C_9H_{18} isomer
43A	154	anisole (tent.)
44	156	C_9H_{18} isomer
44A	157	isopropylbenzene
44B	157	$C_{10}H_{22}$ isomer
45	159	$C_{10}H_{22}$ isomer
46	160	C_9H_{18} isomer
46A	162	$C_{10}H_{20}$ isomer
46B	162	*n*-propylbenzene
47	163	benzaldehyde
47A	163	phenol
48	164	ethyltoluene isomer + unknown
49	165	$C_{11}H_{24}$ isomer + 1,3,5-trimethylbenzene
50	166	$C_{10}H_{22}$ isomer
50A	167	$C_{10}H_{20}$ isomer
51	168	*o*-ethyltoluene
52	169	*n*-octanal

(continued)

Table B18 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
52A	170	$C_{10}H_{20}$ isomer	72A	206	C_5-alkyl benzene isomer
53	170	1,2,4-trimethylbenzene	72B	206	$C_{12}H_{24}$ isomer
54	171	n-decane	72C	207	C_5H_9-benzene isomer
54A	173	isobutylbenzene + dichlorobenzene isomer	73	208	$C_{13}H_{28}$ isomer
54B	174	C_4-alkyl benzene isomer	74	209	$C_{12}H_{24}$ isomer
54C	174	$C_{11}H_{24}$ isomer	75	212	$C_{13}H_{26}$ isomer
54D	175	C_4-alkyl benzene isomer	76	213	C_6-alkyl cyclohexane isomer
55	176	$C_{11}H_{24}$ isomer	77	215	$C_{13}H_{28}$ isomer
55A	176	1,2,3-trimethylbenzene	78	217	unknown
56	178	o-dichlorobenzene	79	218	C_6-alkyl benzene + $C_{13}H_{26}$ isomers
56A	179	indan	80	220	n-tridecane
56B	179	$C_{10}H_{20}$ isomer	80A	221	$C_{13}H_{26}$ isomer
56C	180	C_4-alkyl benzene + $C_{11}H_{24}$ isomers	80B	222	$C_{14}H_{28}$ isomer
57	180	C_4-alkyl benzene + $C_{11}H_{22}$ isomers	81	223	β-methylnaphthalene
58	181	C_4-alkyl benzene isomer	81A	223	$C_{14}H_{30}$ isomer
58A	182	n-butylbenzene	82	225	α-methylnaphthalene
59	182	acetophenone	83	226	unknown
60	184	C_4-alkyl benzene isomer	83A	227	$C_{14}H_{28}$ isomer
60A	184	$C_{11}H_{24}$ isomer	84	229	$C_{14}H_{28}$ isomer
61	186	C_4-alkyl benzene isomer	85A	233	$C_{14}H_{28}$ isomer
61A	186	$C_{11}H_{22}$ isomer	85B	234	biphenyl
62	187	n-nonanal	86	235	n-tetradecane
62A	188	C_4H_7-benzene isomer	86A	237	$C_{15}H_{30}$ isomer
62B	188	$C_{11}H_{22}$ isomer	86B	238	C_2-alkyl naphthalene isomer
63	189	n-undecane	86C	240	dimethylnaphthalene isomer
63A	190	C_5-alkyl benzene isomer	87	isothermal	dimethyl isophthalate (tent.)
63B	191	C_4-alkyl benzene isomer	87A		dimethylnaphthalene isomer
64	191	$C_{11}H_{22}$ isomer	87B		$C_{15}H_{30}$ isomer
65	193	tetramethylbenzene isomer	88		$C_{15}H_{32}$ isomer
65A	194	$C_{12}H_{26}$ isomer	90		$C_{15}H_{30}$ isomer
65B	194	dimethylphenol isomer	91		n-pentadecane
66	195	diethyl maleate	91A		acenaphthene
67	196	unknown	93		dibenzofuran
68	197	C_2-alkyl phenol + C_4H_7-benzene isomers	95		diethyl phthalate
69	199	unknown	97		n-hexadecane
71	204	n-decanal	97A		$C_{16}H_{32}$ isomer (tent.)
72	205	n-dodecane + naphthalene	99		benzophenone
			101		$C_{15}H_{30}O$ isomer
			102		n-heptadecane
			103		$C_{17}H_{34}$ isomer

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B19. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P2/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2A	51	butene isomer
2B	52	butane (tent.)
3	53	acetaldehyde
3A	57	unknown
4	62	isopentane
4B	63	C_5H_{10} isomer
4C	64	furan or C_5H_8 isomer
4D	65	C_5H_{10} isomer
5	65	n-pentane
5A	66	C_5H_8 isomer
5B	67	propanal (tent.) + dimethyl ether
5C	68	C_5H_{10} isomer + dichloromethane
6	69	acetone + acrylonitrile
7	72	isopropanol
7A	77	ter-butanol (tent.)
8	78	2-methylpentane
8A	80	butenal
9	81	3-methylpentane
9A	82	C_6H_{12} isomer
10	83	hexafluorobenzene (es)
10A	84	butanal
11	85	n-hexane
11A	86	chloroform + C_6H_{12} isomer
11B	87	methyl vinyl ketone
11C	88	methyl ethyl ketone
12	90	perfluorotoluene (es)
13	92	methylcyclopentane or C_6H_{12} isomer
13A	94	1,1,1-trichloroethane
13B	97	C_6H_{10} isomer
14	98	benzene
14A	98	C_7H_{16} isomer
14B	99	carbon tetrachloride (tent.)
14C	100	C_7H_{14} isomer
15	100	2-methylhexane
16	101	2,3-dimethylpentane
17	103	3-methylhexane
17A	103	C_7H_{14} isomer
18	105	C_7H_{14} isomer
19	106	trichloroethylene + C_7H_{14} isomer
20	108	n-heptane
20A	110	acetic acid (tent.)
20B	111	C_7H_{14} isomer
20C	114	C_8H_{18} isomer
21	115	methylcyclohexane
21A	116	C_8H_{18} isomer
22	117	2,3-dithiabutane
22A	121	C_8H_{16} isomer
22B	121	C_8H_{18} isomer (tent.)
23	123	toluene
23A	124	C_8H_{18} isomer
24	126	C_8H_{18} isomer
25	128	C_8H_{18} isomer
25A	130	C_8H_{16} isomer
26	131	n-octane
26A	133	C_8H_{16} isomer
27	134	tetrachloroethylene
28	138	C_9H_{20} isomer
28A	140	C_9H_{18} isomer
29	141	chlorobenzene
29A	142	C_9H_{18} isomer
30	144	ethylbenzene
30A	145	C_9H_{20} iosmer
31	146	xylene isomer
32	147	C_9H_{20} isomer
32A	149	styrene or cyclooctatetraene
32B	150	C_9H_{18} isomer
33	150	o-xylene
33A	151	cyclohexanone
34	152	n-nonane
35	153	ketone isomer (tent.)
36	157	isopropylbenzene
36A	159	$C_{10}H_{22}$ isomer
37	160	C_9H_{18} isomer
38	162	benzaldehyde
38A	163	n-propylbenzene
38B	163	$C_{10}H_{22}$ isomer
38C	164	ethyltoluene isomer
39	164	unknown
39A	165	$C_{10}H_{22}$ isomer
40	165	1,3,5-trimethylbenzene
40A	166	$C_{11}H_{24}$ isomer (tent.)
41	166	$C_{10}H_{20}$ isomer
42	168	o-ethyltoluene
42A	168	$C_{10}H_{18}$ isomer (tent.)
43	169	n-octanal + $C_{10}H_{20}$ isomer
44	170	1,2,4-trimethylbenzene
45	171	n-decane
45A	175	C_4-alkyl benzene

(continued)

Table B19 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
45B	175	$C_{11}H_{24}$ isomer
46	176	1,2,3-trimethylbenzene
46A	178	dichlorobenzene isomer
47	179	indan + $C_{10}H_{20}$ isomer
47A	180	C_4-alkyl benzene isomer
48	181	propyltoluene isomer
49	182	*n*-butylbenzene + C_4-alkyl benzene isomer
50	183	acetophenone
50A	184	$C_{11}H_{24}$ isomer
51	184	C_4-alkyl benzene isomer
51A	185	$C_{11}H_{22}$ isomer
52	186	C_4-alkyl benzene isomer
53	188	*n*-nonanal
53A	188	C_4H_7 benzene isomer
54	189	*n*-undecane
54A	190	C_5-alkyl benzene isomer
54B	191	C_4-alkyl benzene + $C_{11}H_{22}$ isomers
54C	192	$C_{12}H_{26}$ isomer
54D	193	tetramethylbenzene isomer
55	195	diethyl maleate
56	197	C_4H_7 benzene + $C_{12}H_{24}$ isomers
57	199	diethyl fumarate
58	200	unknown
58A	201	C_5-alkyl benzene isomer
59	202	C_5-alkyl benzene isomer
60	205	*n*-decanal
61	206	naphthalene + *n*-dodecane
61A	207	$C_{12}H_{24}$ isomer
62	208	$C_{13}H_{28}$ isomer
62A	211	$C_{12}H_{24}$ isomer (tent.)
63	214	$C_{13}H_{26}$ isomer
64	216	$C_{13}H_{26}$ isomer
65	218	$C_{13}H_{28}$ isomer (tent.)
66	221	*n*-tridecane
67	223	β-methylnaphthalene
68	226	α-methylnaphthalene
69	229	$C_{14}H_{28}$ isomer
71	234	$C_{15}H_{30}$ isomer
72	235	*n*-tetradecane

---

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B20. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P2/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2A	50	C_4H_{10} isomer
2B		butene isomer
2C	54	n-butane
3	54	acetaldehyde
4	62	isopentane
4B	64	C_5H_{10} isomer
4C	65	furan
4D	65	C_5H_{10} isomer
5	66	n-pentane
5A	67	propanal
5C	68	C_5H_{10} isomer
5D	69	dichloromethane
5E	70	acetone
6A	74	isopropanol (tent.)
6B	76	ter-butanol
7	78	2-methylpentane
7A	80	butenal isomer (tent.)
8	81	3-methylpentane
8A	82	C_6H_{12} isomer
9	83	hexafluorobenzene (eS)
10	85	n-hexane
10A	86	methyl ethyl ketone
11	86	chloroform
11A	88	C_6H_{12} isomer
12	90	perfluorotoluene (eS)
13	92	methylcyclopentane
13A	92	C_7H_{16} isomer
14	94	1,1,1-trichloroethane
14A	97	C_6H_{10} isomer
15	98	benzene
15A	98	carbon tetrachloride
15B	99	cyclohexane
16	100	2-methylhexane
17	101	2,3-dimethylpentane
18	102	3-methylhexane
19	105	C_7H_{14} isomer
20	106	trichloroethylene
20A	107	C_7H_{14} isomer
21	108	n-heptane
21A	109	C_7H_{14} isomer
21B	110	acetic acid
21C	112	C_7H_{14} isomer
22	115	methylcyclohexane
22A	116	C_8H_{16} isomer
23	116	C_8H_{18} isomer
24	118	C_8H_{16} isomer
24A	119	4-methyl-2-pentanone
25	120	C_8H_{18} isomer
26	122	toluene
26A	123	C_8H_{18} isomer
27	125	C_8H_{18} isomer
28	127	dimethylcyclohexane isomer
28A	128	C_8H_{16} isomer
28B	129	C_8H_{16} isomer
29	130	n-octane
29A	132	dimethylcyclohexane isomer
30	132	tetrachloroethylene
30A	133	C_8H_{16} isomer
31	136	C_9H_{20} isomer (tent.)
32	137	C_9H_{20} isomer
32A	138	C_8H_{16} isomer
33	139	C_9H_{20} isomer
33A	139	ethylcyclohexane
34	141	C_9H_{18} isomer
34A	141	cyclopentanone
34B	142	C_9H_{18} isomer
35	143	ethylbenzene
35A	144	C_9H_{18} isomer
35B	144	C_9H_{20} isomer
36	145	xylene isomer
37	146	C_9H_{20} isomer
37A	148	C_9H_{20} isomer (tent.)
37B	149	styrene
37C	149	C_9H_{18} isomer
38	150	o-xylene
38A	151	C_3-alkyl cyclohexane isomer
39	151	n-nonane
39A	152	alkyl butyrate (tent.)
39B	153	1-acetoxy-butene-1 (tent.)
40	155	C_9H_{18} isomer
40A	156	isopropylbenzene
40B	157	$C_{10}H_{22}$ isomer
40C	158	C_9H_{18} isomer
40D	158	C_9H_{16} isomer
41	159	$C_{10}H_{22}$ isomer
41A	160	propylcyclohexane
41B	160	$C_{10}H_{22}$ isomer
41C	161	$C_{10}H_{20}$ isomer
41D	162	n-propylbenzene
42	163	benzaldehyde
42A	163	ethyltoluene isomer

(continued)

Table B20 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
42B	164	$C_{10}H_{22}$ isomer
43	165	1,3,5-trimethylbenzene
43A	165	$C_{10}H_{22}$ isomer
43B	166	$C_{10}H_{20}$ isomer
43C	167	cyanobenzene (tent.)
44	167	*o*-ethyltoluene
44A	169	$C_{10}H_{20}$ isomer
44B	169	*n*-octanal (tent.)
45	170	1,2,4-trimethylbenzene
46	171	*n*-decane
46A	172	diethyl phthalate
46B	173	$C_{10}H_{20}$ isomer
46C	173	dichlorobenzene isomer
46D	174	C_4-alkyl benzene isomer
46E	175	C_4-alkyl benzene isomer
46F	175	$C_{11}H_{24}$ isomer
47	176	1,2,3-trimethylbenzene
47A	176	$C_{12}H_{26}$ isomer
48	178	*o*-dichlorobenzene
48A	179	indan
48B	179	C_4-alkyl cyclohexane isomer
48C	180	C_4-alkyl benzene + $C_{11}H_{22}$ isomers
49	180	C_4-alkyl benzene isomer
50	181	C_4-alkyl benzene isomer
50A	182	$C_{11}H_{24}$ isomer (tent.)
51	182	acetophenone
51A	183	$C_{11}H_{24}$ isomer
51B	184	C_4-alkyl benzene isomer
52	186	C_4-alkyl benzene isomer
52A	187	C_4-alkyl benzene isomer
53	187	*n*-nonanal
53A	188	$C_{11}H_{22}$ isomer
54	189	*n*-undecane
54A	189	alkyl butyrate (tent.)
55	193	tetramethylbenzene isomer
55A	195	$C_{12}H_{26}$ isomer
56	196	C_5-alkyl benzene isomer
57	197	C_5-alkyl cyclohexane isomer
58	200	$C_{12}H_{24}$ isomer
59	201	C_5-alkyl benzene isomer
60	204	*n*-decanal
61	205	*n*-dodecane + naphthalene
61A	206	$C_{13}H_{26}$ isomer
62	208	$C_{13}H_{28}$ isomer
63	214	$C_{13}H_{26}$ isomer
63A	216	$C_{13}H_{26}$ isomer
64	217	$C_{13}H_{28}$ isomer
65	221	*n*-tridecane
66	223	β-methylnaphthalene
66A	226	α-methylnaphthalene
67	229	hydrocarbon
68	233	$C_{14}H_{30}$ isomer
69	235	*n*-tetradecane

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B21. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P2/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
4	50	chloromethane
4A	52	n-butane
4B	52	butene isomer
5	53	acetaldehyde
5A	55	bromomethane (tent.)
5B	57	chloroethane
6	62	isopentane
6B	65	furan
6C	65	C_5H_{10} isomer
7	66	n-pentane
7A	67	propanal
7B	67	C_5H_{10} isomer
8	69	dichloromethane
9	70	acetone
9B	72	carbon disulfide
9C	75	isopropanol (tent.)
9D	77	ter-butanol
10	78	2-methylpentane
10A	80	butanal
10B	81	butenal
11	82	3-methylpentane
11A	83	C_6H_{12} isomer
12	84	hexafluorobenzene (eS)
13	85	n-hexane
14	86	C_6H_{12} isomer + chloroform
14A	87	methyl ethyl ketone
14B	90	C_6H_{12} isomer
15	91	perfluorotoluene (eS)
16	92	methylcyclopentane
16A	93	1,2-dichloroethane
17	94	1,1,1-trichloroethane
17A	97	C_6H_{10} isomer
18	98	benzene
18A	99	carbon tetrachloride
18B	100	cyclohexane
19	101	2-methylhexane
20	102	2,3-dimethylpentane
21	103	3-methylhexane
21A	104	C_6H_{10} isomer
22	105	C_7H_{14} isomer
23	107	trichloroethylene
23A	107	C_7H_{14} isomer
24	108	n-heptane
24A	111	acetic acid (tent.)
25	115	methylcyclohexane
25A	116	C_8H_{10} isomer
26	117	2,3-dithiabutane or $C_2H_6S_2$ isomer
26A	119	C_8H_{16} isomer
27	119	4-methyl-2-pentanone
28	122-6	toluene
29	128	C_8H_{16} isomer
29A	130	C_8H_{16} isomer
30	131	n-octane
30A	132	C_8H_{16} isomer
31	133	tetrachloroethylene
32	137	C_9H_{20} isomer
32A	138	dithiapentane isomer
32B	139	C_9H_{20} isomer
32C	139	C_9H_{18} isomer
33	140	chlorobenzene
34	142	C_9H_{18} isomer
35	144	ethylbenzene
35A	149	C_9H_{20} isomer
36	146	xylene isomer
37	147	C_9H_{20} isomer
38	149	cyclohexanone
39	150	o-xylene
40	152	n-nonane
41	156	3,4-dithiahexane
42	157	isopropylbenzene
42A	157	$C_{10}H_{22}$ isomer
43	159	$C_{10}H_{22}$ isomer
44	160	C_3-alkyl cyclohexane isomer
45	161	$C_{10}H_{18}$ isomer (tent.)
45A	162	$C_{10}H_{20}$ isomer
45B	162	n-propylbenzene
46	163	benzaldehyde
46A	163	phenol
47	164	ethyltoluene isomer
47A	165	unknown
48	165	1,3,5-trimethylbenzene
48A	166	$C_{11}H_{24}$ isomer
48B	167	$C_{10}H_{20}$ isomer
48C	167	cyanobenzene
49	168	o-ethyltoluene
50	170	n-octanal (tent.)
51	170	1,2,4-trimethylbenzene + $C_{10}H_{20}$ isomer
52	171	n-decane
52A	173	$C_{10}H_{20}$ isomer

(continued)

Table B21 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
53	173	dichlorobenzene isomer
53A	175	C_4-alkyl benzene isomer
53B	176	$C_{11}H_{24}$ isomer
54	176	1,2,3-trimethylbenzene
54A	178	tolualdehyde isomer (tent.)
55	178	*o*-dichlorobenzene
55A	179	indan + $C_{11}H_{22}$ isomer
55B	179	C_4-alkyl cyclohexane isomer
55C	180	C_4-alkyl benzene isomer
56	181	propyltoluene isomer
56A	181	cresol isomer
57	182	*n*-butylbenzene + C_4-alkyl benzene isomer
58	182	acetophenone
59	183	$C_{11}H_{24}$ isomer
59A	184	C_4-alkyl benzene isomer
60	185	C_4-alkyl benzene isomer
60A	187	C_4-alkyl benzene isomer
61	187	*n*-nonanal
61A	188	$C_{11}H_{22}$ isomer
62	189	*n*-undecane
62A	191	C_4-alkyl benzene isomer
62B	191	$C_{11}H_{22}$ isomer
62C	192	ethylphenol isomer
62D	193	tetramethylbenzene + $C_{12}H_{24}$ isomers
63	195	dimethylphenol isomer
64	196	diethyl maleate
64A	196	unknown
65	197	C_2-alkyl phenol isomer
66	199	unknown
66A	201	C_3-alkyl phenol isomer
67	202	C_2-alkyl phenol isomer
67A	203	trichlorobenzene isomer
68	204	*n*-decanal
69	205	naphthalene + *n*-dodecane
69A	206	C_5-alkyl benzene isomer
69B	207	$C_{12}H_{24}$ isomer
70	208	$C_{13}H_{28}$ isomer
70A	213	$C_{13}H_{26}$ isomer (tent.)
71	214	C_6-alkyl cyclohexane isomer
72	215	C_5H_9-benzene isomer
73	217	unknown
73A	220	*n*-undecanal
74	221	*n*-tridecane
74A	222	$C_{13}H_{26}$ isomer
75	223	β-methylnaphthalene
76	226	α-methylnaphthalene
77	228	$C_{14}H_{28}$ isomer
78	232	$C_{14}H_{30}$ isomer
78A	234	biphenyl
79	235	*n*-tetradecane
79A	240	C_2-alkyl naphthalene isomer
79B	240	C_2-alkyl naphthalene isomer
79D	240	$C_{15}H_{30}$ isomer
80	240	*n*-pentadecane
80A	240	$C_{16}H_{32}$ isomer
81	240	unknown

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B22. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P3/L4)[a]

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2A	50	chloromethane
2B	51	C_4H_{10} isomer
2C	52	butene isomer
2D	53	*n*-butane (tent.)
3	53	acetaldehyde
4	55	chloroethane
5	61	isopentane
6A	63	C_5H_{10} isomer
6B	63	furan (tent.)
6C	64	propenal
7	64	*n*-pentane
7A	65	propanal
7B	65	C_5H_{10} isomer
7C	67	dichloromethane
8	67	acetone
9A	70	carbon disulfide
9B	75	ter-butanol
10	77	2-methylpentane
10A	78	*n*-butanal (tent.)
10B	79	butenal isomer
11	80	3-methylpentane
11A	81	C_6H_{12} isomer
12	82	hexafluorobenzene (sW)
13	83	*n*-hexane
14	84	chloroform
14A	86	C_6H_{12} isomer
15	88	perfluorotoluene (sW)
16	90	methylcyclopentane
16A	91	methyl ethyl ketone + dichloromethane (tent.)
16B	93	1,1,1-trichloroethane
16C	96	C_6H_{10} isomer
17	97	benzene
17A	97	carbon tetrachloride (tent.)
17B	98	cyclohexane
18	99	2-methylhexane
19	100	2,3-dimethylpentane
20	101	3-methylhexane
21	104	C_7H_{14} isomer
22	105	trichloroethylene
22A	105	acetic acid
23	107	*n*-heptane
23A	108	C_7H_{14} isomer
24	110	C_7H_{14} isomer
24A	113	C_8H_{18} isomer
25	114	methylcyclohexane
25A	115	C_8H_{18} isomer
26	116	2,3-dithiabutane or $C_2H_6S_2$ isomer
26A	118	C_8H_{16} isomer
27	119	4-methyl-2-pentanone
27A	120	C_8H_{16} isomer
28	122	toluene
29	124	C_8H_{18} isomer
30	127	C_8H_{16} isomer
31	128	*n*-hexanal
32	129	*n*-octane
32A	131	C_8H_{16} isomer
33	132	tetrachloroethylene
33A	134	C_8H_{16} isomer
34	136	C_9H_{20} + dithiapentane isomers
35	138	C_9H_{20} isomer
36	139	chlorobenzene
36A	141	C_9H_{18} isomer
37	143	ethylbenzene
37A	144	C_9H_{20} isomer
38	144	xylene isomer
39	145	C_9H_{20} isomer
39A	147	2-heptanone or $C_7H_{14}O$ isomer
40	148	cyclohexanone
41	149	*n*-heptanal
42	150	*o*-xylene
42A	150	C_9H_{18} isomer
43	151	*n*-nonane
44	152	1-acetoxy-butene-1 (tent.)
44A	153	C_9H_{18} isomer
45	155	3,4-dithiahexane
46	156	isopropylbenzene
46A	156	$C_{10}H_{22}$ isomer
47	158	$C_{10}H_{22}$ isomer
48	159	C_3-alkyl cyclohexane isomer
48A	160	$C_{10}H_{22}$ isomer
48B	161	$C_{10}H_{20}$ isomer
49	162	*n*-propylbenzene + benzaldehyde
50	163	ethyltoluene isomer
50A	163	unknown
51	164	1,3,5-trimethylbenzene
51A	165	$C_{10}H_{22}$ isomer
51B	166	cyanobenzene (tent.) + $C_{16}H_{20}$ isomer
52	167	*o*-ethyltoluene

(continued)

Table B22 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
52A	168	$C_{11}H_{24}$ isomer
53	168	*n*-octanal
53A	169	$C_{10}H_{20}$ isomer
54	169	1,2,4-trimethylbenzene
55	170	*n*-decane
55A	172	isobutylbenzene + dichlorobenzene isomer
55B	173	*sec*-butylbenzene
56	174	$C_{10}H_{20}$ + C_4-alkyl benzene isomer
56A	175	$C_{11}H_{24}$ isomer
57	175	1,2,3-trimethylbenzene
57A	177	*o*-dichlorobenzene + $C_{11}H_{24}$ isomer
58	178	indan + $C_{11}H_{22}$ isomer
58A	178	C_4-alkyl cyclohexane isomer
58B	179	C_4-alkyl benzene isomer
59	180	C_4-alkyl benzene isomer
59A	181	cresol isomer
60	181	*n*-butylbenzene + C_4-alkyl benzene isomer
61	182	acetophenone
61A	182	$C_{11}H_{24}$ isomer
62	183	C_4-alkyl benzene isomer
63	185	C_4-alkyl benzene isomer
63A	186	C_4-alkyl benzene isomer
64	187	*n*-nonanal
64A	188	$C_{11}H_{22}$ isomer
65	188	*n*-undecane
66	190	C_4-alkyl benzene + $C_{11}H_{22}$ isomers
66A	192	$C_{12}H_{26}$ isomer
67	193	tetramethylbenzene isomer
67A	194	dimethylphenol isomer
68	195	diethyl maleate
69	195	unknown
69A	196	C_2-alkyl phenol isomer
70	197	$C_{11}H_{22}$ + C_4H_7-benzene isomers
70A	197	C_5-alkyl benzene isomer
71	198	diethyl fumarate
72	199	unknown
73	200	C_5-alkyl benzene isomer
74	201	C_5-alkyl benzene isomer
74A	201	$C_{10}H_{20}O$ isomer (tent.)
74B	202	$C_{12}H_{24}$ isomer
74C	202	trichlorobenzene isomer
75	204	*n*-decanal
76	205	*n*-dodecane + naphthalene
76A	205	C_5-alkyl benzene isomer
76B	206	C_5H_9-benzene isomer
76C	207	$C_{12}H_{24}$ isomer
77	207	$C_{13}H_{28}$ isomer
79	213	$C_{13}H_{26}$ isomer
80A	216	$C_{13}H_{28}$ isomer
81	217	unknown
81A	218	$C_{13}H_{26}$ isomer
82	219	*n*-undecanal
83	220	*n*-tridecane
84	222	β-methylnaphthalene
85	225	α-methylnaphthalene
86	226	unknown
87	228	$C_{14}H_{30}$ isomer (tent.)
87A	231	$C_{15}H_{32}$ isomer
88	232	$C_{14}H_{30}$ isomer
88A	233	$C_{14}H_{28}$ isomer
89	234	*n*-tetradecane
89A	239	biphenyl
89B	240	$C_{14}H_{28}$ isomer (tent.)
89C	240	$C_{15}H_{30}$ isomer
89D	240	C_2-alkyl naphthalene isomer
90	240	$C_{16}H_{34}$ isomer
91A	isothermal	$C_{15}H_{30}$ isomer
92		*n*-pentadecane
92A		$C_{15}H_{24}O$ alcohol isomer (tent.)
92B		acenaphthene
93		unknown
94		diethyl phthalate
95		*n*-hexadecane
96		benzophenone
97		saturated hydrocarbon
98		$C_{15}H_{30}O$ isomer
99		*n*-heptadecane
100		saturated hydrocarbon

---

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B23. VOLATILE ORGANICS IN AMBIENT AIR AT E. I. DuPONT (P4/L4)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2A	50	propane (tent.)
2B	50	chloromethane (tent.)
2C	53	C_4H_8 isomer
2D	53	n-butane
3	54	acetaldehyde
3A	61	isopentane
4A	63	C_5H_{12} isomer
4B	64	furan
4C	65	propenal
5	65	propanal
6	68	dichloromethane + acetone
7A	72	C_3H_8O isomer
7B	77	C_4H_8O aldehyde isomer
8	78	2-methylpentane
8A	79	2-methylpropenal
9	81	3-methylpentane
9A	82	C_6H_{12} isomer
10	83	hexafluorobenzene (eS)
11	84	n-hexane
12	86	chloroform
12A	87	methyl vinyl ketone
12B	88	methyl ethyl ketone
13	89	perfluorotoluene (eS)
14	91	methylcyclopentane
14A	92	1,2-dichloroethane
15	94	1,1,1-trichloroethane
15A	96	C_6H_{10} isomer
16	97	benzene
16A	98	dimethylpentane isomer
16B	99	carbon tetrachloride
16C	99	cyclohexane
17	100	2-methylhexane
18	101	2,3-dimethylpentane
19	102	3-methylhexane
19A	104	3-ethylpentane
20	105	C_7H_{14} isomer
21	106	trichloroethylene
22	107	n-heptane
22A	108	$C_5H_{10}O$ isomer
23	109	methyl methacrylate
23A	111	acetic acid (tent.)
23B	113	C_8H_{18} isomer
24	114	methylcyclohexane
25	116	C_8H_{18} isomer
25A	118	C_8H_{16} isomer
26	118	4-methyl-2-pentanone
26A	120	C_8H_{16} isomer
27	123	toluene
28	125	C_8H_{18} isomer
28A	127	C_8H_{16} isomer
28B	129	hexanal (tent.)
29	129	1,2-dibromoethane
30	130	n-octane
31	133	tetrachloroethylene
31A	136	C_9H_{20} isomer
31B	139	C_9H_{20} isomer
32	140	chlorobenzene
33	144	ethylbenzene
34	145	xylene isomer
34A	146	C_9H_{20} isomer
34B	147	C_9H_{18} isomer
34C	148	C_9H_{20} isomer
34D	149	styrene
35	150	o-xylene
35A	151	C_9H_{18} isomer
36	152	n-nonane
36A	154	C_9H_{18} isomer
37	157	isopropylbenzene
37A	159	$C_{10}H_{22}$ isomer
37B	160	C_9H_{18} isomer
38	161	2-methylcyclohexanone
38A	162	n-propylbenzene
39	163	benzaldehyde
40	163	phenol
40A	164	ethyltoluene isomer
41	165	$C_{10}H_{22}$ + C_3-alkyl benzene isomers
42	166	cyanobenzene + methylpyridine or aniline
42A	168	C_3-alkyl benzene isomer
43	169	n-octanal
44	170	1,2,4-trimethylbenzene
45	171	n-decane
45A	173	diethyl phthalate (tent.)
46	173	dichlorobenzene isomer
47	176	C_4-alkyl benzene isomer
47A	177	$C_{11}H_{24}$ isomer
48	178	o-dichlorobenzene
48A	180	$C_{11}H_{24}$ isomer
48B	181	cresol isomer
48C	181	C_4-alkyl benzene isomer

(continued)

Table B23 (cont'd)

Chromatographic[a] Peak No.	Elution Temp. (°C)	Compound
49	182	acetophenone
50	183	cresol + $C_{11}H_{24}$ isomers
50A	185	C_4-alkyl benzene isomer
51	186	nitrobenzene
51A	187	C_4-alkyl benzene isomer
52	187	*n*-nonanal
52A	188	$C_{11}H_{22}$ isomer
53	189	*n*-undecane
54	189	C_5-alkyl benzene isomer
54A	191	alkyl isobutyrate (tent.)
55	193	chloroaniline isomer
55A	194	nitrophenol isomer
56	195	dichlorotoluene or $C_7H_6Cl_2$ isomer
56A	196	$C_9H_{13}N$ isomer (tent.)
58	198	*o*-nitrotoluene
59	200	$C_{12}H_{24}$ isomer + benzoic acid (tent.)
61	203	trichlorobenzene isomer
62	204	*n*-decanal
63	205	naphthalene + *n*-dodecane
64	208	*p*-nitrotoluene
65	210	trichlorobenzene isomer
66	210	chloronitrobenzene isomer
67	212	chloronitrobenzene isomer
68	214	$C_{13}H_{26}$ isomer
69	217	$C_{14}H_{30}$ isomer
70	221	*n*-tridecane
71	223	β-methylnaphthalene
72	225	dichloronitrobenzene or dichloroaniline isomer
73	226	α-methylnaphthalene
73A	227	$C_{14}H_{28}$ isomer
74	229	dichloronitrobenzene or dichloroaniline isomer
75	233	$C_{14}H_{30}$ isomer
76	234	biphenyl
77	235	*n*-tetradecane
78	237	dimethylnaphthalene isomer
78A	239	$C_{14}H_{28}$ isomer
78B	240	alkyl phthalate (tent.)
78C	240	$C_{16}H_{34}$ isomer
78D	240	$C_{15}H_{30}$ isomer
79	240	*n*-pentadecane

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B24. VOLATILE ORGANICS IN AMBIENT AIR AT E. I. DuPONT (P5/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2A	52	*n*-propane (tent.)
2B	53	butene (tent.)
3	54	acetaldehyde
3A	55	*n*-butane (tent.)
3B	61	isopentane
3D	64	C_5H_{10} isomer
3E	65	*n*-pentane
3F	66	propenal + propanal
4	67	dichloromethane
5	69	diethyl ether
5A	70	acetone
6	78	2-methylpentane
6A	79	C_4H_8O isomer (tent.)
6B	80	2-methylpropenal
6C	81	3-methylpentane
7	83	hexafluorohexane (eS)
8	84	*n*-hexane
9	86	chloroform
9A	86	butanal (tent.)
9B	88	methyl vinyl ketone
9C	89	methyl ethyl ketone
10	89	perfluorotoluene (eS)
11	91	methylcyclopentane
11A	93	1,2-dichloroethane (tent.)
11B	94	1,1,1-trichloroethane
12	97	benzene + C_7H_{16} isomer
12A	98	carbon tetrachloride
12B	98	cyclohexane
13	99	2-methylhexane
14	100	2,3-dimethylpentane
15	101	3-methylhexane
15A	103	C_7H_{14} isomer
16	104	3-ethylpentane
17	105	C_7H_{14} isomer
17A	105	trichloroethylene (tent.)
17B	106	*n*-pentanal
18	107	*n*-heptane
18A	108	acetic acid
19	110	C_7H_{14} isomer
20	112	C_8H_{18} isomer
21	113	methylcyclohexane
22	115	C_8H_{18} isomer
22A	117	C_8H_{16} isomer
23	118	4-methyl-2-pentanone
23A	119	C_8H_{16} isomer (tent.)
24	121	toluene
24A	122	C_8H_{18} isomer
25	124	C_8H_{18} isomer
26	126	C_8H_{16} isomer
27	128	*n*-hexanal + C_8H_{16} isomer
28	129	*n*-octane
28A	131	C_8H_{16} isomer
29	132	tetrachloroethylene
29A	136	C_9H_{18} isomer
29B	138	C_9H_{20} isomer
30	139	chlorobenzene
30A	140	C_9H_{18} isomer
31	142	ethylbenzene isomer
31A	143	C_9H_{20} isomer
32	144	xylene isomer
32A	145	C_9H_{20} isomer
32B	148	styrene
33	149	*o*-xylene
33A	149	C_9H_{18} isomer + *n*-heptanal (tent.)
34	150	*n*-nonane
34A	154	C_9H_{18} isomer
34B	155	$C_{10}H_{22}$ isomer (tent.)
34C	160	*n*-propylbenzene
35	161	benzaldehyde
36	162	phenol
36A	163	ethyltoluene isomer
37	164	$C_{10}H_{22}$ isomer + 1,3,5-trimethylbenzene
37A	165	cyanobenzene
37B	166	C_3-alkyl benzene isomer
37C	166	$C_8H_{16}O$ isomer
37D	167	$C_{10}H_{22}$ isomer
38	168	*n*-octanal
39	169	1,2,4-trimethylbenzene
40	170	*n*-decane
40A	171	$C_{10}H_{20}$ isomer
41	172	dichlorobenzene isomer
41A	174	1,2,3-trimethylbenzene + C_4-alkyl benzene isomer
42	175	$C_{11}H_{24}$ isomer (tent.)
42A	176	phenylacetaldehyde
43	177	*o*-dichlorobenzene
43A	178	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
44	179	cresol isomer

(continued)

Table B24 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
44A	180	C_4-alkyl benzene isomer
45	181	acetophenone
46	182	$C_{11}H_{24}$ isomer
47	184	C_4-alkyl benzene + $C_9H_{18}O$ isomers
48	186	*n*-nonanal
49	187	*n*-undecane
49A	189	$C_{11}H_{22}$ isomer
49B	190	C_2-alkyl phenol isomer (tent.)
49C	191	C_4-alkyl benzene isomer
50	192	dimethylphenol isomer
50A	194	C_5-alkyl benzene + $C_{11}H_{22}$ isomers (tent.)
51	195	C_2-alkyl phenol isomer
52	197	$C_{12}H_{24}$ (tent.) + C_2-alkyl phenol + $C_9H_{10}O$ isomers
52A	199	C_3-alkyl phenol isomer
53	200	$C_{10}H_{20}O$ isomer
54	202	*n*-decanal
55	203	*n*-dodecane + naphthalene
55A	205	$C_{12}H_{24}$ isomer
56	212	$C_{12}H_{24}$ isomer
57	215	$C_{13}H_{28}$ isomer
58	218	*n*-undecanal
59	219	*n*-tridecane
60	221	β-methylnaphthalene
60A	223	α-methylnaphthalene
62	230	alkyl butyrate
62A	232	$C_{15}H_{32}$ isomer (tent.)
63	233	*n*-tetradecane
67	240	*n*-pentadecane
68	240	unknown

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B25. VOLATILE ORGANICS IN AMBIENT AIR AT E. I. DuPONT (P5/L4)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	46	CO_2
2A	50	propane (tent.)
2B	52	butene
3	53	acetaldehyde
3A	54	n-butane (tent.)
3B	55	C_5H_{10} isomer
3C	59	isopentane
5	63	propanal + n-pentane (tent.)
5A	64	C_5H_{10} isomer
6	65	acetone
6A	66	dichloromethane
7	74	2-methylpentane
7A	75	2-methylpropenal
8	77	3-methylpentane
8A	78	n-butanal
9	79	hexafluorobenzene (es)
10	80	n-hexane
11	82	chloroform
12	85	perfluorotoluene (es)
13	88	methylcyclopentane
13A	88	methyl ethyl ketone
13B	89	1,2-dichloroethane
13C	90	1,1,1-trichloroethane
14	94	benzene + 3,3-dimethylpentane
14A	95	carbon tetrachloride
14B	95	cyclohexane
15	96	2-methylhexane
16	97	2,3-dimethylpentane
17	98	3-methylhexane
18	101	3-ethylpentane + C_7H_{14} isomer
19	102	C_7H_{14} isomer + trichloroethylene
20	104	n-heptane
20A	105	n-pentanal
20B	106	acetic acid (tent.)
21	107	C_8H_{16} isomer
22	110	C_8H_{18} isomer
23	111	methylcyclohexane
24	112	C_8H_{18} isomer
25	115	C_8H_{16} isomer
25A	116	4-methyl-2-pentanone
26	117	C_8H_{16} isomer (tent.)
27	119	toluene
27A	120	C_8H_{18} isomer
28	122	C_8H_{18} isomer
29	125	C_8H_{16} isomer
30	126	1,2-dibromoethane
30A	127	n-hexanal
31	127	n-octane
32	130	tetrachloroethylene
32A	136	C_8H_{16} isomer
33	137	chlorobenzene
33A	138	C_9H_{18} isomer
34	141	ethylbenzene
34A	141	C_9H_{18} isomer
35	142	xylene isomer
35A	144	$C_{10}H_{22}$ isomer
35B	146	styrene
36	148	o-xylene
36A	148	C_9H_{18} isomer
37	149	n-nonane
37A	154	isopropylbenzene
37B	155	$C_{10}H_{20}$ isomer
39	161	benzaldehyde + phenol
39A	162	ethyltoluene isomer
40	163	1,3,5-trimethylbenzene
40A	163	$C_{10}H_{22}$ isomer
41	164	cyanobenzene + $C_{10}H_{20}$ isomer
41A	165	C_3-alkyl benzene isomer
42	167	n-octanal
42A	168	$C_{10}H_{20}$ isomer
43	168	1,2,4-trimethylbenzene
44	169	n-decane
44A	170	$C_{10}H_{20}$ isomer
45	171	dichlorobenzene isomer
46	174	C_4-alkyl benzene isomer
47	176	o-dichlorobenzene
48	179	cresol isomer
48A	179	C_4-alkyl benzene isomer
49	180	acetophenone
49A	183	C_4-alkyl benzene isomer
50	184	nitrobenzene
51	185	n-nonanal
52	187	n-undecane
52A	188	C_5-alkyl benzene isomer
53	193	dichlorotoluene + dimethylphenol isomers
54	195	C_2-alkyl phenol isomer
55	197	$C_{12}H_{24}$ isomer (tent.)
56	200	$C_{12}H_{24}$ isomer
56A	201	C_3-alkyl phenol isomer
57	202	trichlorobenzene isomer

(continued)

Table B25 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
58	203	n-decanal
59	204	naphthalene + n-dodecane
60	206	$C_{12}H_{24}$ isomer
61	208	trichlorobenzene isomer
61A	209	chloronitrobenzene isomer
62	210	chloronitrobenzene isomer
63	212	$C_{13}H_{26}$ isomer
64	213	$C_{12}H_{24}$ isomer
65	214	$C_{13}H_{26}$ isomer (tent.)
66	218	n-undecanal
67	219	n-tridecane
68	221	β-methylnaphthalene + $C_{13}H_{26}$ isomers
68A	224	α-methylnaphthalene
69	227	dichloronitrobenzene or dichloroaniline isomer
70	231	$C_{14}H_{30}$ isomer (tent.)
71	232	biphenyl + $C_{14}H_{28}$ isomer
72	233	n-tetradecane
73	235	diphenyl ether
74	238	alkyl phthalate (BKG)
75A	240	$C_{15}H_{30}$ isomer
76	240	n-pentadecane
77	240	unknown

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B26. VOLATILE ORGANICS IN AMBIENT AIR AT E. I. DuPONT (P6/L1)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2A	50	butene
3	51	acetaldehyde
3A	53	*n*-butane (tent.)
3B	57	isopentane (tent.)
3C	59	furan
4	60	propenal + C_5H_{10} isomer
4A	60	propenal + *n*-pentane
5	63	acetone
5A	63	dichloromethane (tent.)
6A	71	2-methylpentane
6B	72	2-methylpropenal
6C	74	3-methylpentane
7	76	hexafluorobenzene (eT)
8	78	*n*-hexane
8A	79	chloroform
8B	80	*n*-butanal (tent.)
9	82	perfluorotoluene (eT)
9A	84	C_7H_{16} isomer
9B	85	methylcyclopentane
9C	87	1,1,1-trichloroethane (tent.)
9D	89	benzene
10	91	3,3-dimethylpentane
10A	92	carbon tetrachloride
10B	93	cyclohexane
11	93	2-methylhexane
12	94	2,3-dimethylpentane
13	95	3-methylhexane
14	98	3-ethylpentane
15	99	C_7H_{14} isomer + trichloroethylene (tent.)
15A	100	*n*-pentanal
16	101	*n*-heptane
16A	106	C_8H_{18} isomer
17	108	methylcyclohexane
17A	109	C_8H_{18} isomer
17B	110	C_8H_{16} isomer
18	116	toluene
18A	117	C_8H_{16} isomer
19	119	C_8H_{18} isomer
19A	124	*n*-hexanal
20	125	*n*-octane
21	128	tetrachloroethylene
21A	131	C_8H_{16} isomer
22	135	chlorobenzene
23	139	ethylbenzene
24	141	xylene isomer
24A	142	phenylacetylene (tent.)
24B	145	styrene (tent.)
24C	145	C_9H_{18} isomer
25	146	*o*-xylene + *n*-heptanal
26	148	*n*-nonane
26A	153	isopropylbenzene (tent.)
26B	154	$C_{10}H_{22}$ isomer
27	158	benzaldehyde
28	159	phenol
28A	160	ethyltoluene isomer
29	161	$C_{10}H_{22}$ isomer
29A	163	cyanobenzene
29B	164	$C_{11}H_{24}$ isomer (tent.)
30	166	*n*-octanal
30A	167	1,2,4-trimethylbenzene + $C_{10}H_{20}$ isomer
31	168	*n*-decane
31A	170	dichlorobenzene isomer
32	173	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
32A	174	phenylacetaldehyde
33	175	*o*-dichlorobenzene
34	178	cresol isomer
35	179	acetophenone
36	181	$C_{11}H_{24}$ isomer (tent.)
37	183	$C_{11}H_{22}$ + C_4-alkyl benzene isomers
38	184	*n*-nonanal
38A	185	$C_{11}H_{22}$ isomer
39	186	*n*-undecane
39A	187	$C_{12}H_{24}$ isomer
39B	189	ethylphenol isomer
39C	191	C_4-alkyl benzene isomer
40	191	dimethylphenol isomer
40A	193	$C_{11}H_{22}$ isomer
41	195	dimethylphenol isomer
42	196	*o*-nitrotoluene
43	199	C_3-alkyl phenol isomer
43A	200	trichlorobenzene isomer
44	201	*n*-decanal
45	203	*n*-dodecane
46	205	$C_{12}H_{24}$ + C_3-alkyl phenol isomers (tent.)
47	209	unknown
48	211	$C_{12}H_{24}$ isomer

(continued)

Table B26 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
49	213	$C_{13}H_{28}$ isomer
50	217	_n_-undecanal
51	218	_n_-tridecane
52	226	$C_{14}H_{30}$ isomer (tent.)
54	233	_n_-tetradecane

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B27. VOLATILE ORGANICS IN AMBIENT AIR AT E. I. DuPONT (P6/L2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	44	CO_2
2A	51	butene
2B	51	n-butane
3	52	acetaldehyde
3A	59	isopentane (tent.)
4A	61	furan + C_5H_{10} isomer
4B	62	propenal
5	63	propanal + n-pentane
5A	64	C_5H_{10} isomer
5B	65	dichloroethylene isomer
5C	65	dichloromethane
6	66	acetone
7A	68	C_6H_{14} isomer
7B	73	butanal
8	75	2-methylpentane
8A	76	2-methylpropenal
8B	77	C_6H_{12} isomer
9	78	3-methylpentane
10	80	hexafluorobenzene (eB)
11	81	n-hexane
12	83	chloroform
13	86	perfluorotoluene (eB)
13A	86	C_7H_{16} isomer
14	87	methylcyclopentane
15	90	1,1,1-trichloroethane
15A	92	C_6H_{10} isomer
15B	93	benzene
16	94	C_7H_{16} isomer
16A	94	carbon tetrachloride
16B	95	cyclohexane
17	97	2-methylhexane
18	98	2,3-dimethylpentane
19	99	3-methylhexane
20	102	3-ethylpentane
21	103	C_7H_{14} isomer
22	105	n-heptane
22A	106	C_7H_{16} isomer
22B	107	acetic acid (tent.)
22C	110	C_8H_{18} isomer
22D	111	C_8H_{18} isomer
23	111	methylcyclohexane
24	113	C_8H_{18} isomer
25	119	toluene
25A	120	C_8H_{18} isomer
26	122	C_8H_{18} isomer
27	128	n-octane
28	130	tetrachloroethylene
28A	135	cyclopentanone
28B	136	C_9H_{20} isomer
29	137	chlorobenzene
30	141	ethylbenzene
31	143	xylene isomer
32	144	C_9H_{20} isomer
32A	147	styrene
32B	148	n-heptanal
33	148	o-xylene
33A	149	C_9H_{18} isomer
34	150	n-nonane
34A	152	C_9H_{18} isomer
34B	153	isopropylbenzene
34C	154	$C_{10}H_{22}$ isomer
35	160	benzaldehyde
36	161	phenol
36A	162	ethyltoluene isomer
37	163	$C_{10}H_{22}$ isomer
38	164	cyanobenzene
39A	165	C_3-alkyl benzene isomer
39	167	n-octanal
40	168	1,2,4-trimethylbenzene
40A	168	$C_{10}H_{20}$ isomer
41	169	n-decane
42	171	dichlorobenzene (tent.) + C_4-alkyl benzene isomers
42A	171	$C_{10}H_{20}$ isomer
42B	172	C_4-alkyl benzene isomer
43	173	1,2,3-trimethylbenzene
43A	174	$C_{11}H_{24}$ isomer
43B	175	phenylacetaldehyde
44	176	o-dichlorobenzene
44A	176	indan
45	178	cresol isomer
45A	179	C_4-alkyl benzene isomer
46	180	acetophenone
47	182	$C_{11}H_{24}$ isomer
48	184	C_4-alkyl benzene isomer
48A	185	$C_{11}H_{22}$ isomer
49	186	n-nonanal
50	187	n-undecane
50A	189	C_4-alkyl benzene isomer
50B	190	ethylphenol isomer
51	191	chloroaniline or chloromethyl-pyridine isomer

(continued)

Table B27 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
51A	191	C_4-alkyl benzene isomer
52	192	dimethylphenol isomer
53	195	C_2-alkyl phenol isomer
54	197	C_4H_7-benzene isomer
54A	198	C_5-alkyl benzene isomer
55	200	C_3-alkyl phenol + $C_{12}H_{24}$ isomers
56	202	*n*-decanal
57	203	naphthalene
58	206	2,3-benzothiophene
60	212	$C_{12}H_{24}$ isomer
61	213	quinoline
62	219	$C_{13}H_{26}$ isomer (tent.)
63	220	*n*-tridecane
63A	221	methylbenzothiophene isomer
64	222	β-methylnaphthalene
64A	223	methylquinoline isomer
65	224	α-methylnaphthalene
65A	226	alkyl phthalate (tent.)
66	227	$C_{14}H_{28}$ isomer
67	231	butyl butyrate
68	232	biphenyl
69	233	*n*-tetradecane
70	236	ethylnaphthalene isomer
71	238	dimethylnaphthalene isomer
72	240	dimethylnaphthalene isomer
73	isothermal	dimethylnaphthalene isomer
74		biphenylene
74A		$C_{15}H_{30}$ isomer
75		*n*-pentadecane + methylbiphenyl isomer
75A		methylbiphenyl isomer (tent.)
76		acenaphthene
77		C_3-alkyl naphthalene isomer
78		dibenzofuran
78A		C_3-alkyl naphthalene isomer
81		fluorene
83		4-phenyl-benzaldehyde (tent.)
84		$C_{13}H_{10}O$ isomer

---

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B28. VOLATILE ORGANICS IN AMBIENT AIR AT E. I. DuPONT (P6/L8)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	45	CO_2
2A	51	propane (tent.)
2B	54	butene isomer
2C	55	butane
3	56	acetaldehyde
3A	60	C_5H_{12} isomer
3B	64	isopentane
3D	66	furan
3E	66	C_5H_{10} isomer
3F	67	*n*-pentane
3G	69	propanal
3H	70	bromoethane + propenal
3I	70	dichloromethane
3K	73	dimethyl ether (tent.)
3L	74	methylpropanal isomer
3M	75	acetone
3N	80	2-methylpentane
3O	83	3-methylpentane
4	85	hexafluorobenzene (eS)
5	86	*n*-hexane
5A	87	*n*-butanal
5B	88	chloroform
6	91	perfluorotoluene (eS)
6A	93	methylcyclopentane
6B	94	methyl ethyl ketone
6C	96	1,1,1-trichloroethane
7	99	benzene
7A	99	C_7H_{16} isomer
7B	100	carbon tetrachloride
7C	101	cyclohexane
8	101	2-methylhexane
8A	102	2,3-dimethylpentane
9	103	3-methylhexane
10	106	C_7H_{14} isomer
10A	107	trichloroethylene (tent.)
11	109	*n*-heptane
11A	110	*n*-pentanal
11B	110	acetic acid (tent.)
12	111	methyl methacrylate
12A	114	C_8H_{18} isomer (tent.)
13	115	methylcyclohexane
13A	116	C_8H_{16} isomer
13B	116	C_8H_{18} isomer
13C	120	4-methyl-2-pentanone
14	123	toluene
14A	124	C_8H_{18} isomer
14B	125	C_8H_{18} isomer
14C	128	C_8H_{16} isomer
14D	129	C_8H_{18} isomer
15	130	1,2-dibromoethane
15A	131	*n*-hexanal
16	131	*n*-octane
16A	132	2-hexanone
17	133	tetrachloroethylene
17A	138	C_9H_{20} isomer
17B	139	C_9H_{20} isomer
18	140	chlorobenzene
19	143	ethylbenzene
19A	144	C_9H_{20} isomer
20	145	xylene isomer
20A	146	C_9H_{20} isomer
20B	147	C_9H_{18} isomer
20C	148	3-heptanone
20D	149	2-heptanone + styrene
20E	149	*n*-heptanal
21	150	*o*-xylene
22	151	*n*-nonane
22A	153	C_9H_{18} isomer
23	156	isopropylbenzene
23A	156	$C_{10}H_{22}$ isomer
23B	157	$C_{10}H_{22}$ isomer
23C	159	C_9H_{18} isomer
23D	160	$C_{11}H_{24}$ isomer
24	160	$C_8H_{16}O$ ketone
24A	161	2-methylcyclohexanone (tent.)
24B	161	*n*-propylbenzene
25	162	benzaldehyde
25A	162	phenol
25B	163	ethyltoluene isomer
25C	163	$C_{10}H_{22}$ isomer
26	168	$C_{11}H_{24}$ isomer + 1,3,5-trimethylbenzene
26A	166	cyanobenzene
27	167	C_3-alkyl benzene + octanone isomers
28	168	*n*-octanal
28A	169	$C_{10}H_{20}$ isomer
29	169	1,2,4-trimethylbenzene
30	170	*n*-decane
31	172	triisobutylene
31A	172	dichlorobenzene isomer
32	173	$C_{12}H_{24}$ isomer (tent.)

(continued)

Table B28 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
32A	174	$C_{11}H_{24}$ isomer
33	175	C_4-alkyl benzene isomer
33A	176	$C_{11}H_{24}$ isomer
34	177	*o*-dichlorobenzene
35	179	C_4-alkyl benzene isomer
35A	180	cresol + C_4-alkyl benzene isomers
36	181	acetophenone
37	182	$C_{11}H_{22}$ + $C_{11}H_{24}$ isomers
37A	184	C_4-alkyl benzene isomer
38	184	nitrobenzene
38A	186	C_4-alkyl benzene isomer
39	187	*n*-nonanal
39A	188	$C_{11}H_{22}$ isomer
40	188	*n*-undecane
40A	189	C_5-alkyl benzene isomer
40B	190	$C_{11}H_{22}$ isomer
40C	192	chlorobenzaldehyde isomer
40D	192	chloroaniline isomer
40E	193	C_4-alkyl benzene isomer
40F	193	dimethylphenol isomer
41	194	*o*-nitrophenol
41A	194	dichlorotoluene isomer
41B	195	$C_{11}H_{20}$ isomer (tent.)
41C	196	$C_9H_{11}N$ isomer (tent.)
42	196	C_2-alkyl phenol + $C_{11}H_{22}$ isomers
43	198	*o*-nitrotoluene
44	199	C_4-alkyl benzene + $C_{12}H_{26}$ isomers
44A	200	C_5-alkyl benzene isomer
45	200	$C_{12}H_{24}$ isomer
45A	201	C_3-alkyl phenol isomer
46	202	trichlorobenzene isomer
47	203	*n*-decanal
48	204	naphthalene + *n*-dodecane
48A	205	$C_{12}H_{24}$ isomer
48B	206	$C_{13}H_{26}$ isomer
59	207	nitrotoluene *p* or *m*
50	208	trichlorobenzene isomer
51	209	chloronitrobenzene isomer
51A	209	$C_{13}H_{26}$ isomer
52	210	chloronitrobenzene isomer
53	212	$C_{12}H_{24}$ isomer
53A	213	$C_{13}H_{26}$ isomer
54	216	$C_{14}H_{30}$ isomer
54A	217	$C_{11}H_{22}O$ isomer
55	218	*n*-undecanal
56	219	*n*-tridecane
56A	220	$C_{13}H_{26}$ isomer
57	221	β-methylnaphthalene
57A	222	$C_{14}H_{28}$ isomer
58	224	α-methylnaphthalene
58A	226	$C_{14}H_{28}$ isomer (tent.)
59	227	dichloronitrobenzene or dichloroaniline isomer
60	231	alkyl butyrate
61	232	biphenyl
62	233	*n*-tetradecane
62A	234	$C_{14}H_{28}$ isomer
63	235	diphenyl ether
63A	238	dimethylnaphthalene isomer
64	240	dimethylnaphthalene isomer
65	240	$C_{15}H_{32}$ isomer (tent.)
66	240	*n*-pentadecane
67	240	acenaphthene
68	240	dibenzofuran
69	240	diethyl phthalate
70	240	*n*-hexadecane + 2,2,4-trimethyl-penta-1,3-diol di-isobutyrate

[a] See Table 30 for protocol. An OV-101 SCOT was used.

Table B29. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P1/L1)^{a}a

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	93	CO_2
1A	94	C_6H_{14} isomer
1B	95	C_7H_{16} isomer
1C	95	hexafluorobenzene (e[illegible]) + perfluorotoluene (e[illegible])
1D	96	C_8H_{18} isomer
1E	97	n-octane
1F	97	C_9H_{20} isomer
1G	98	C_8H_{16} isomer
2	98	C_8H_{16} isomer
3	100	n-nonane
3A	101	dichloromethane + $C_{10}H_{22}$ isomer
3B	101	C_9H_{18} isomer
4	102	benzene
4A	103	C_9H_{18} isomer
4B	103	$C_{10}H_{20}$ isomer
5	104	n-decane
5A	105	$C_{11}H_{24}$ isomer
6	105	chloroform
6A	106	$C_{10}H_{20}$ isomer
6B	106	tetrachloroethylene
6C	107	$C_{11}H_{24}$ isomer
7	108	toluene
8	109	n-undecane
8A	110	$C_{11}H_{22}$ isomer
9	111	$C_{12}H_{26}$ isomer
10	112	ethylbenzene
11	113	xylene isomer
11A	114	$C_{12}H_{26}$ isomer
11B	114	$C_{10}H_{18}$ isomer
11C	115	$C_{11}H_{22}$ isomer
11D	115	$C_{12}H_{24}$ isomer
11E	116	C_3-alkyl benzene isomer
11F	117	$C_{13}H_{26}$ isomer
12	118	o-xylene
13	119	n-propylbenzene
14	122	ethyltoluene isomer
14A	123	C_4-alkyl benzene + $C_{13}H_{26}$ isomers
15	124	trimethylbenzene isomer
15A	125	n-tridecane
15B	126	$C_{14}H_{30}$ isomer
16	126	C_3-alkyl benzene isomer
16A	127	C_4-alkyl benzene isomer
16B	128	$C_{14}H_{28}$ isomer (tent.)
17	129	trimethylbenzene isomer
17A	130	n-octanal
17B	130	1-acetoxy-butene-1 (tent., (BKG)
18	131	C_4-alkyl benzene isomer
18A	132	$C_{14}H_{28}$ isomer
19	132	C_4-alkyl benzene isomer
20	134	C_4-alkyl benzene isomer
20A	134	C_5-alkyl benzene isomer
20B	135	C_4-alkyl benzene isomer
20C	135	C_4-alkyl benzene isomer
21	136	trimethylbenzene isomer
22	137	C_4-alkyl benzene isomer
23	138	C_4-alkyl benzene isomer
23A	139	$C_{15}H_{30}$ isomer
24	139	C_4-alkyl benzene isomer
24A	140	C_5-alkyl benzene isomer
25	141	C_3H_5-benzene isomer
25A	142	$C_9H_{18}O$ ketone + C_5-alkyl benzene isomers
26	142	n-nonanal
26A	143	C_5-alkyl benzene isomer
27	144	C_4H_7-benzene isomer
27A	144	C_5-alkyl benzene isomer
27B	145	C_4-alkyl benzene + $C_{15}H_{32}$ isomers
27B	146	C_5-alkyl benzene isomer
28	147	C_4-alkyl benzene isomer
28A	148	$C_{15}H_{30}$ isomer
29	149	C_4-alkyl benzene isomer
29A	151	unsaturated hydrocarbon
30	153	$C_{16}H_{34}$ isomer
30A	154	C_4H_7-benzene isomer
30B	155	$C_{10}H_{20}O$ ketone isomer
31	156	n-decanal
32	158	C_5H_9-benzene isomer
32A	159	C_5-alkyl benzene isomer
33	162	benzaldehyde
34	165	C_6-alkyl benzene + C_5H_9-benzene isomers (tent.)
34A	167	saturated hydrocarbon
35	169	n-undecanal
35A	171	C_5H_9-benzene isomer
36	174	unsaturated hydrocarbon
37	177	acetophenone
37A	178	C_6H_{11}-benzene isomer (tent.)

(continued)

Table B29 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
39	186	unknown
40	188	naphthalene
41	193	unsaturated hydrocarbon (tent.)
41A	198	alkyl butyrate (BKG)
42	200	methylnaphthalene isomer
43	203	methylnaphthalene isomer
44	208	hydrocarbon
45	213	phenol
46	216	alkyl ketone (tent.)
46A	217	C_2-alkyl naphthalene isomer
47	220	dimethylphenol isomer
47A	221	cresol isomer
49	230	C_2-alkyl phenol isomer

[a] See Table 30 for protocol. A Carbowax 20 M SCOT was used.

Table B30. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P1/L2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	93	CO_2
2	94	n-heptane + hexafluorobenzene (eE) + perfluorotoluene (eE)
3	96	n-octane
3A	97	C_8H_{16} isomer
4	97	C_9H_{20} isomer
5	98	n-nonane
5A	99	$C_{10}H_{22}$ isomer
6	100	benzene
6A	101	C_9H_{18} isomer
7	102	n-decane + trichloroethylene (tent.)
8	103	$C_{10}H_{20}$ isomer
9	104	tetrachloroethylene
9A	105	$C_{11}H_{24}$ isomer
10	106	toluene
10A	107	$C_{11}H_{22}$ isomer
11	108	$C_{12}H_{26}$ isomer
12	110	C_2-alkyl benzene isomer
12A	110	$C_{12}H_{26}$ isomer
13	111	C_2-alkyl benzene isomer
13A	111	$C_{12}H_{24}$ isomer
13B	112	$C_{12}H_{24}$ isomer
13C	113	$C_{14}H_{30}$ isomer
14	114	xylene isomer
15	115	n-propylbenzene
15A	116	$C_{11}H_{20}$ isomer
16	117	C_3-alkyl benzene isomer
16A	118	$C_{13}H_{26}$ isomer
16B	119	n-tridecane
17	120	C_3-alkyl benzene isomer
17A	121	$C_{13}H_{26}$ isomer
17B	122	C_4-alkyl benzene isomer
18	122	C_3-alkyl benzene isomer
18A	127	$C_{14}H_{30}$ isomer
19	125	C_3-alkyl benzene isomer
20	126	n-octanal + C_4-alkyl benzene isomer
21	127	1-acetoxy-butene-1 (tent.)
21A	128	C_4-alkyl benzene isomer
21B	129	$C_{14}H_{28}$ isomer
22	130	C_4-alkyl benzene isomer
23	131	cyclohexanone
23A	132	C_4-alkyl benzene isomer
24	133	C_3-alkyl benzene isomer
25	134	n-tetradecane
26	135	C_4-alkyl benzene isomer
27	136	C_5-alkyl benzene isomer
27A	137	C_4-alkyl benzene isomer
27B	138	$C_{14}H_{28}$ isomer
28	139	C_3H_5-benzene isomer
28A	139	C_5-alkyl benzene isomer
29	140	n-nonanal
30	141	C_5-alkyl benzene + C_4H_7-benzene isomers
31	143	C_4-alkyl benzene isomer
31A	143	C_5-alkyl benzene isomer
31B	144	$C_{16}H_{32}$ isomer
32	145	C_4-alkyl benzene isomer
32A	146	C_5-alkyl benzene isomer
33	147	C_4-alkyl benzene isomer
33A	148	$C_{15}H_{30}$ isomer
34	149	saturated hydrocarbon
35A	151	C_6-alkyl benzene isomer
36	152	saturated hydrocarbon
37	153	C_4H_7-benzene isomer
38	154	n-decanal
38A	155	dichlorobenzene + $C_{16}H_{34}$ isomer
39	156	C_4H_7-benzene isomer
39A	157	C_5H_9-benzene isomer
39B	157	C_5-alkyl benzene isomer
39C	158	$C_{15}H_{32}$ isomer
40	160	benzaldehyde
41	161	unknown
42	163	unsaturated hydrocarbon
44	167	n-undecanal
45	169	unknown
45A	171	cyanobenzene
45B	173	unsaturated hydrocarbon
46	173	diethyl fumarate
47	176	acetophenone
48A	179	$C_{17}H_{36}$ isomer
49	180	$C_{17}H_{34}$ isomer
50	185	unknown
51	186	diethyl maleate
52	187	naphthalene
53A	191	$C_{18}H_{38}$ isomer
54	195	unknown
55A	199	alkyl butyrate (BKG)
56	201	methylnaphthalene isomer
57	205	methylnaphthalene isomer

(continued)

Table B30 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
58	208	unsaturated hydrocarbon (tent.)
59	212	phenol
59A	214	biphenyl (tent.)
60	215	alkyl ketone
60A	217	C_2-alkyl naphthalene isomer
61	220	C_2-alkyl phenol isomer
62	221	cresol isomer
63	227	C_2-alkyl phenol isomer
64	230	C_2-alkyl phenol isomer
65	231	acenaphthene
67	240	dibenzofuran

[a] See Table 30 for protocol. A Carbowax 20 M SCOT was used.

Table B31. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P1/L4)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	93	CO_2
1A	94	C_7H_{16} isomer
2	95	hexafluorobenzene (eI) + perfluorotoluene (eI)
2A	95	C_8H_{18} isomer
3	96	*n*-octane
3A	97	C_8H_{16} isomer
4	98	C_9H_{20} isomer
5	99	*n*-nonane
6	100	dichloromethane
6A	100	$C_{10}H_{22}$ isomer
7	101	benzene
7A	102	C_9H_{18} isomer
8	103	*n*-decane
8A	104	chloroform
9	105	$C_{10}H_{20}$ isomer + tetrachloroethylene
10	107	toluene
10A	107	$C_{11}H_{24}$ isomer
11	109	$C_{11}H_{22}$ isomer
12	111	ethylbenzene
13	112	xylene isomer
13A	113	$C_{12}H_{26}$ isomer
13B	113	$C_{10}H_{18}$ isomer (tent.)
13C	114	isopropylbenzene
14	116	*o*-xylene
15	119	*n*-propylbenzene
16	120	chlorobenzene
16A	121	C_3-alkyl benzene isomer
17	123	trimethylbenzene isomer
17A	124	*n*-tridecane
17B	125	$C_{13}H_{26}$ isomer
18	125	C_3-alkyl benzene isomer
18A	126	C_4-alkyl benzene isomer
18B	127	$C_{12}H_{24}$ isomer
19	128	trimethylbenzene isomer
19A	129	*n*-octanal
19B	129	1-acetoxy-butene-1 (tent.)
20	130	C_4-alkyl benzene isomer
20A	131	C_4-alkyl benzene isomer
20B	132	$C_{13}H_{26}$ isomer
20C	133	C_4-alkyl benzene isomer
21	133	cyclohexanone
21A	134	C_4-alkyl benzene isomer
22	135	trimethylbenzene + $C_{13}H_{26}$ isomers
23	136	C_4-alkyl benzene isomer
23A	136	*n*-tetradecane
24	137	C_4-alkyl benzene isomer
25	138	C_5-alkyl benzene + C_4-alkyl benzene isomers
25A	139	unsaturated hydrocarbon
26	140	C_3H_5-benzene isomer
27	142	*n*-nonanal
27A	142	C_5-alkyl benzene isomer
28	143	C_4H_7-benzene + C_5-alkyl benzene isomers
28A	145	C_4-alkyl benzene isomer
28B	145	C_5-alkyl benzene isomer
29	146	C_4-alkyl benzene + $C_{15}H_{30}$ isomers
29A	147	$C_{15}H_{28}$ + C_5-alkyl benzene isomers
30	148	C_4-alkyl benzene isomer
30A	149	C_5-alkyl benzene isomer
31	149	saturated hydrocarbon
32	152	$C_{15}H_{32}$ isomer
33	154	C_4H_7-benzene isomer
34	155	*n*-decanal
34A	156	C_5-alkyl benzene isomer
34B	157	$C_{16}H_{30}$ isomer
35	158	C_4H_7-benzene isomer
35A	159	C_5-alkyl benzene isomer
35B	159	C_5H_9-benzene isomer
36	161	benzaldehyde
37	162	unknown
38	164	unsaturated hydrocarbon + C_6-alkyl benzene isomer
39	167	*n*-hexadecane
40	169	*n*-undecanal
41	170	unknown
41A	171	cyanobenzene
41B	172	C_6H_{11}-benzene isomer (tent.)
42	174	diethyl fumarate
42A	176	unsaturated hydrocarbon
43	177	acetophenone
44	179	*n*-heptadecane
44A	182	unsaturated hydrocarbon
45	186	unknown
46	187	diethyl maleate
47	188	naphthalene
48	191	$C_{18}H_{38}$ isomer

(continued)

Table B31 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
49	195	unknown
49A	197	unsaturated hydrocarbon
50	198	alkyl butyrate isomer
51A	201	methylnaphthalene isomer
52	203	$C_{15}H_{24}O$ isomer
53	205	methylnaphthalene isomer
54	207	acrylamide
54A	212	dimethylnaphthalene isomer
55	213	phenol
56A	215	C_2-alkyl naphthalene isomer
57	216	dimethylnaphthalene isomer
58	220	C_2-alkyl phenol isomer
59	221	cresol isomer
60	223	C_3-alkyl phenol isomer
62	227	C_3-alkyl naphthalene isomer (tent.)
63	231	C_2-alkyl phenol isomer
64	232	N,N-dimethylbenzamide

[a] See Table 30 for protocol. A Carbowax 20 M SCOT was used.

Table B32. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P1/L2)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	93	CO_2
2	94	n-hexane
3	95	C_7H_{16} isomer + hexafluorobenzene (eM) + perfluorotoluene (eM)
3A	96	C_7H_{14} isomer
3B	97	C_8H_{18} isomer
4	97	C_8H_{16} isomer
4A	98	C_9H_{18} isomer
4B	99	1,1,1-trichloroethane
5	99	n-nonane
6	100	methyl ethyl ketone
6A	100	dichloromethane (tent.)
6B	101	$C_{10}H_{22}$ isomer
7	102	benzene
7A	103	C_9H_{18} isomer
8	104	trichloroethylene + n-decane
9	105	chloroform
9A	106	$C_{10}H_{20}$ isomer
10	106	tetrachloroethylene
10A	107	$C_{11}H_{24}$ isomer
11	108	toluene
11A	109	$C_{11}H_{24}$ isomer
11B	110	$C_{11}H_{22}$ isomer
12	111	$C_{12}H_{26}$ isomer
12A	111	$C_{11}H_{22}$ isomer
13	112	ethylbenzene
14	113	xylene isomer + n-dodecane
14A	114	$C_{10}H_{18}$ isomer (tent.)
14B	114	$C_{11}H_{22}$ isomer
14C	115	isopropylbenzene
14D	116	$C_{12}H_{24}$ isomer
15	117	o-xylene
15A	118	$C_{13}H_{28}$ isomer
15B	118	$C_{13}H_{26}$ isomer
16	119	n-propylbenzene
17	121	ethyltoluene isomer
18	124	trimethylbenzene isomer + n-tridecane
18A	125	C_4-alkyl benzene isomer
19	126	styrene + C_3-alkyl benzene isomer
19A	127	C_4-alkyl benzene isomer
19B	127	$C_{14}H_{28}$ isomer
20	129	trimethylbenzene isomer
20A	129	n-octanal
21	130	1-acetoxy-butene-1 (tent.)
21A	131	C_4-alkyl benzene isomer
21B	133	C_4-alkyl benzene isomer
22	134	cyclohexanone
22A	135	$C_{14}H_{28}$ + C_4-alkyl benzene isomers
23	136	trimethylbenzene isomer
23A	137	C_4-alkyl benzene isomer
24	138	n-tetradecane
25	139	C_4-alkyl benzene + unsaturated hydrocarbon isomers
25A	140	C_3H_5-benzene isomer
26	143	n-nonanal
26A	148	C_4-alkyl benzene isomer
26B	148	C_5-alkyl benzene isomer
27	149	C_4-alkyl benzene + $C_{14}H_{28}$ isomers
27A	150	$C_{15}H_{32}$ isomer
28	150	$C_8H_{18}O$ (tent.) + dichlorobenzene isomers (tent.)
29	153	$C_{16}H_{34}$ isomer (tent.)
29A	155	C_4H_7-benzene isomer
30	156	n-decanal
30A	157	dichlorobenzene isomer
30B	158	C_4H_7-benzene isomer
31	159	$C_{15}H_{30}$ isomer
32	162	benzaldehyde
32A	163	unknown
33	163	$C_{13}H_{30}$ isomer
34	165	unsaturated hydrocarbon
36	168	n-hexadecane
37	169	n-undecanal (tent.)
38	170	unknown
38A	172	cyanobenzene
38B	174	unsaturated hydrocarbon
38C	174	dodecanal (tent.)
39	175	diethyl fumarate
39A	175	$C_{17}H_{34}$ isomer
41	178	acetophenone
42	180	n-heptadecane
43	187	unknown
44	189	naphthalene
44A	194	$C_{18}H_{38}$ isomer (tent.)
45	197	unknown
46	199	unsaturated hydrocarbon

(continued)

Table B32 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
47	202	2,2,4-trimethyl-penta-1,3-diol di-isobutyrate
48	203	methylnaphthalene isomer
49	206	methylnaphthalene isomer
50	209	saturated hydrocarbon (tent.)
53	214	phenol
53A	216	biphenyl
53B	218	C_2-alkyl naphthalene isomer
54	220	C_2-alkyl phenol isomer
55	221	C_2-alkyl phenol isomer
56	223	cresol isomer
57	224	C_3-alkyl phenol isomer
58	227	tri-butyl phosphate (tent.)
59	228	C_2-alkyl phenol isomer
60	231	C_2-alkyl phenol isomer
60A	232	acenaphthene (tent.)
61	235	C_6-alkyl phenol isomer

---

[a] See Table 30 for protocol. A Carbowax 20 M SCOT was used.

Table B33. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P2/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	93	CO_2
2	94	n-hexane
3	95	n-heptane + hexafluorobenzene (e■) + perfluorotoluene (e■)
3A	96	C_8H_{18} isomer
4	97	n-octane
4A	97	C_8H_{16} isomer
5	98	C_9H_{20} isomer
5A	99	C_9H_{18} isomer
6	99	n-nonane
6A	100	C_9H_{18} isomer
6B	100	$C_{10}H_{22}$ isomer
7	101	benzene
7A	102	trichloroethylene
7B	103	$C_{10}H_{20}$ isomer
8	103	n-decane
8A	104	tetrachloroethylene
9	105	toluene
9A	107	$C_{11}H_{24}$ isomer
9B	108	$C_{11}H_{22}$ isomer
10	110	ethylbenzene
11	111	$C_{12}H_{26}$ + xylene isomers
11A	111	$C_6H_8N_2$ isomer (tent.)
12	113	isopropylbenzene
13	115	o-xylene
14	117	n-propylbenzene
14A	118	3,4-dithiahexane
15	119	ethyltoluene isomer
16	122	trimethylbenzene isomer
16A	122	$C_{13}H_{28}$ isomer
16B	124	C_4-alkyl benzene isomer (tent.)
17	124	C_3-alkyl benzene isomer + styrene (tent.)
17A	125	C_4-alkyl benzene isomer
18	127	trimethylbenzene isomer
19	128	1-acetoxy-butene-1
19A	129	C_4-alkyl benzene isomer
20	130	$C_{13}H_{26}$ + C_4-alkyl benzene isomers
20A	131	C_4-alkyl benzene isomer
21	132	cyclohexanone
21A	133	C_4-alkyl benzene isomer
22	135	trimethylbenzene isomer
23	136	C_4-alkyl benzene isomer
24	137	$C_{14}H_{30}$ + C_4-alkyl benzene isomers
25	138	C_4-alkyl benzene isomer
25A	139	C_3H_5-benzene isomer
26	141	n-nonanal
27	143	saturated hydrocarbon (tent.) + C_5-alkyl benzene isomer
27A	145	C_5-alkyl benzene isomer
28	146	C_4-alkyl benzene isomer
29	147	C_4-alkyl benzene isomer
30	148	dichlorobenzene isomer + unknown
31	152	$C_{15}H_{30}$ isomer (tent.)
32	154	n-decanal
32A	155	dichlorobenzene isomer
33	157	C_4H_7-benzene isomer
34	160	benzaldehyde isomer
35	161	unknown
36	164	unsaturated hydrocarbon
37	165	C_6-alkyl benzene isomer (tent.)
38	168	unsaturated hydrocarbon
39	169	$C_{13}H_{10}O_2$ isomer (tent.)
39A	171	cyanobenzene
40	173	diethyl fumarate
41	174	unsaturated hydrocarbon
42	176	acetophenone
43	179	$C_{17}H_{36}$ isomer
43A	180	$C_{17}H_{34}$ isomer
44	186	diethyl maleate
45	188	naphthalene
45A	190	$C_{18}H_{38}$ isomer
46	195	unknown
47	197	unsaturated hydrocarbon
49	200	alkyl butyrate + cresol isomer
50	201	methylnaphthalene isomer
50A	204	methylnaphthalene isomer
50B	212	cresol isomer
51	213	phenol
51A	217	C_2-alkyl naphthalene isomer
51B	221	C_2-alkyl phenol isomer
51C	222	cresol isomer

---

[a] See Table 30 for protocol. A Carbowax 20 M SCOT was used.

Table B34. VOLATILE ORGANICS IN AMBIENT AIR AT AMERICAN CYANAMID CORP. (P3/L3)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	93	CO_2
1A	94	n-pentane + acetaldehyde (tent.)
1B	94	diethyl ether + n-hexane
2	95	C_7H_{16} isomer + hexafluorobenzene (es) + perfluorotoluene (es)
2A	96	C_8H_{16} isomer
2B	96	C_7H_{14} isomer
3	97	n-octane
3A	98	C_8H_{16} isomer
3B	98	C_9H_{20} isomer
3C	99	dichloromethane
4	99	n-nonane
5	100	benzene
6	101	$C_{10}H_{22}$ + C_9H_{18} isomers
7	102	$C_{10}H_{22}$ isomer
8	103	chloroform
8A	104	$C_{11}H_{24}$ isomer
8B	104	n-decane
8C	105	tetrachloroethylene + $C_{10}H_{20}$ isomer
9	106	toluene
10	108	n-undecane
10A	109	$C_{11}H_{22}$ isomer
10B	110	$C_{11}H_{22}$ isomer
10C	110	$C_{12}H_{26}$ isomer
10D	111	ethylbenzene
11	112	xylene isomer
12	114	$C_{12}H_{26}$ isomer
12A	115	C_3-alkyl benzene isomer
13	116	o-xylene
14	119	n-propylbenzene
15	121	C_3-alkyl benzene isomer
16	123	C_3-alkyl benzene isomer
16A	124	C_4-alkyl benzene isomer
16B	124	$C_{13}H_{26}$ isomer
16C	125	C_4-alkyl benzene isomer
17	126	C_3-alkyl benzene isomer
17A	127	$C_{13}H_{28}$ isomer
18	129	trimethylbenzene isomer
19	130	C_4-alkyl benzene isomer
19A	131	$C_{13}H_{28}$ isomer
19B	131	C_4-alkyl benzene isomer
20	132	cyclohexanone
21	133	C_4-alkyl benzene isomer
21A	134	C_5-alkyl benzene isomer (tent.)
21B	135	C_4-alkyl benzene isomer
22	136	trimethylbenzene isomer
23	137	C_4-alkyl benzene + $C_{14}H_{28}$ isomers
24	138	C_4-alkyl benzene isomer
25	139	C_4-alkyl benzene isomer
25A	140	C_5-alkyl benzene isomer
26	140	C_4-alkyl benzene + C_3H_5-benzene isomers
26A	141	$C_{14}H_{26}$ isomer
27	142	C_5-alkyl benzene isomer
27A	143	n-tetradecane
27B	143	C_4H_7-benzene isomer
27C	144	C_5-alkyl benzene + $C_{15}H_{30}$ isomers
27D	145	C_4-alkyl benzene isomer
27E	146	C_5-alkyl benzene isomer
28	147	C_4-alkyl benzene isomer
28A	148	C_5-alkyl benzene isomer
29	149	C_4-alkyl benzene isomer
30	150	$C_{15}H_{32}$ isomer
30A	151	C_5-alkyl benzene isomer
31	151	C_4-alkyl benzene isomer + saturated hydrocarbon
31A	152	C_6-alkyl benzene isomer
31B	153	$C_{15}H_{30}$ isomer
32	154	C_4H_7-benzene isomer
32A	155	n-pentadecane
32B	155	C_5H_9-benzene isomer
33	156	C_5-alkyl benzene + $C_{17}H_{34}$ isomers
34	158	C_5H_9-benzene + C_6-alkyl benzene isomers
34A	159	C_4H_7-benzene isomer
34B	160	C_5-alkyl benzene isomer
35	161	benzaldehyde
36	161	unknown
37	166	C_6-alkyl benzene isomer
37A	167	unsaturated hydrocarbon
38	170	unknown
38A	172	C_5H_9-benzene isomer
38B	173	o-tolualdehyde (tent.)
39	174	diethyl fumarate
39A	175	$C_{17}H_{34}$ + C_5H_9-benzene isomers

(continued)

Table B34 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
40	177	acetophenone
41	185	unknown
42	187	diethyl maleate
43	189	naphthalene
45	195	unknown
46	198	unknown
47	201	methylnaphthalene isomer
49	205	methylnaphthalene isomer
49A	209	$C_{14}H_{10}O$ isomer (tent.)
50	213	phenol
50A	217	dimethylphenol isomer
51	220	C_2-alkyl phenol isomer
52	221	cresol isomer
53	227	C_2-alkyl phenol isomer
54	230	C_2-alkyl phenol isomer

[a] See Table 30 for protocol. A Carbowax 20 M SCOT was used.

Part III

Camden, NJ-Philadelphia, PA

Table B35. VOLATILE ORGANICS IDENTIFIED IN AIR IN BRISTOL, PA (P1/LLA)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	54	C_4H_8 isomer
3	55	acetaldehyde
3A	56	*n*-butane (tent.)
4	63	acetone
4A	66	methylene chloride
5A	73	2-methylpentane
6	77	hexafluorobenzene (eI)
6A	78	*n*-hexane
6B	79	methyl ethyl ketone
7	82	perfluorotoluene (eI)
7A	83	C_7H_{16} isomer
7B	83	1,2-dichloroethane
8	85	1,1,1-trichloroethane
8A	87	benzene
9	88	C_6H_{16} isomer
9A	88	carbon tetrachloride (traces)
9B	89	cyclohexane
10	90	2-methylhexane
11	91	2,3-dimethylpentane
12	92	3-methylhexane
12A	94	C_7H_{14} isomer
13	95	3-ethylpentane
13A	96	C_7H_{14} isomer
14	97	*n*-heptane
14A	101	C_8H_{18} isomer
15	102	methylcyclohexane
15A	103	C_8H_{18} isomer
16	104	acetic acid
17	106	C_8H_{18} isomer
18	109	toluene
18A	110	C_8H_{18} isomer
19	112	C_8H_{18} isomer
20	117	*n*-octane
21	119	tetrachloroethylene
21A	122	C_8H_{16} isomer
22	128	ethylbenzene
23	130	xylene isomer
23A	132	C_9H_{20} isomer
23B	134	styrene
24	135	*o*-xylene
25	137	*n*-nonane
25A	143	isopropylbenzene
26	145	benzaldehyde
26A	146	*n*-propylbenzene
27	147	ethyltoluene isomer
27A	148	C_3-alkyl benzene isomer + benzonitrile
28	149	phenol
28A	151	C_3-alkyl benzene isomer
29	152	*n*-octanal
30	153	1,2,4-trimethylbenzene
31	155	*n*-decane
31A	156	C_3-alkyl benzene isomer
31B	159	C_4-alkyl benzene isomer
32	161	$C_{11}H_{22}$ isomer
32A	163	C_4-alkyl benzene isomer
33	164	acetophenone
33A	165	cresol + $C_{11}H_{24}$ isomers
33B	168	C_4-alkyl benzene isomer
33C	169	$C_{12}H_{24}$ isomer
33D	169	C_4-alkyl benzene isomer
34	170	*n*-nonanal
34A	171	$C_{11}H_{22}$ isomer
35	172	*n*-undecane
35A	175	C_4-alkyl benzene isomer
36	177	C_2-alkyl phenol isomer
37	180	C_2-alkyl phenol isomer
37A	182	C_2-alkyl phenol + $C_{12}H_{24}$ isomers
37B	184	C_4-alkyl benzene isomer
37C	185	C_3-alkyl phenol isomer
38	186	naphthalene
38A	187	*n*-decanal + $C_{12}H_{24}$ isomer
39	188	*n*-dodecane
39A	200	C_3-alkyl phenol isomer
40	202	*n*-tridecane
40A	203	β-methylnaphthalene
40B	203	$C_{13}H_{26}$ isomer
40C	205	α-methylnaphthalene
41	212	alkyl butyrate
41A	213	$C_{14}H_{30}$ isomer
42	216	*n*-tetradecane
43	217	$C_{12}H_{18}O_2$ isomer (tent.)
43A	220	C_2-alkyl naphthalene isomer
44	221	$C_{15}H_{30}$ isomer
46	229	*n*-pentadecane
47	231	unknown
49A	240	*n*-hexadecane
52	240	alkyl phenol
53	240	*n*-heptadecane
54	240	sat. hydrocarbon

---

[a] See Table 31 for protocol.

Table B36. VOLATILE ORGANICS IDENTIFIED IN AIR IN BRISTOL, PA (P1/LLB)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2	51	isobutane
2A	51	C_4H_8 isomer
2B	52	n-butane
2C	53	C_4H_8 isomer
2D	54	acetaldehyde
3	59	acetone
3A	62	dichloroethylene isomer (traces)
4	63	methylene chloride
5A	67	C_4H_8O isomer (tent.)
6	70	2-methylpentane
7	72	3-methylpentane
7A	73	methyl ethyl ketone
8	74	hexafluorobenzene (eI)
9	75	n-hexane
9A	76	ethyl acetate
10	80	C_7H_{16} isomer + perfluorotoluene (eI)
11	81	C_7H_{16} isomer + methylcyclopentane
12	82	1,1,1-trichloroethane
13	85	benzene
13A	86	C_7H_{16} isomer
14	87	cyclohexane
15	87	2-methylhexane
15A	88	2,3-dimethylpentane
16	89	3-methylhexane
16A	91	C_7H_{14} isomer
17	91	3-ethylpentane
17A	92	C_7H_{14} isomer
18	92	C_8H_{18} isomer + trichloroethylene (traces)
18A	93	2,5-dimethylfuran
19	94	n-heptane
20	96	2,5-dimethyltetrahydrofuran
21	98	acetic acid
22	99	methylcyclohexane
23	101	C_8H_{18} isomer
24	103	$C_6H_{12}O$ isomer (tent.)
25	107	toluene
25A	108	C_8H_{18} isomer (tent.)
26	109	3-hexanone
27	110	2-hexanone
27A	111	C_8H_{16} isomer
28	112	C_8H_{18} isomer
29	113	tertiary amyl alcohol
30	114	alcohol isomer (tent.)
31	115	n-octane
32	116	tetrachloroethylene
32A	119	C_8H_{16} isomer (tent.)
33	122	chlorobenzene
34	126	ethylbenzene
34A	127	C_9H_{18} isomer
35	127	xylene isomer
36	129	C_9H_{20} isomer
37	130	butyl acrylate
38	131	styrene
39	132	o-xylene
39A	133	C_9H_{18} isomer
40	134	n-nonane
40A	135	C_8H_{14} isomer
40B	136	dimethylpyrrole isomer (tent.)
41	137	C_8H_{14} isomer or unknown
41A	138	isopropylbenzene
42	143	benzaldehyde
42A	144	n-propylbenzene
42B	145	C_9H_{18} isomer
43	145	ethyltoluene isomer
44	146	benzonitrile
44A	147	phenol
45	148	C_8H_{10} isomer
45A	149	C_3-alkyl benzene isomer
45B	151	$C_7H_{14}O$ isomer (tent.)
45C	151	benzofuran
47	153	n-decane
48	154	dichlorobenzene isomer
48A	157	C_4-alkyl benzene + trimethylbenzene isomers
48B	157	$C_{11}H_{24}$ isomer
48C	158	dichlorobenzene isomer
49	159	unknown
49A	161	C_4-alkyl benzene isomer
50	162	acetophenone
51	164	$C_{11}H_{24}$ isomer
52	166	C_4-alkyl benzene isomer
53	167	methyl benzoate
54	168	n-nonanal
54A	169	$C_{11}H_{22}$ isomer
55	170	n-undecane
55A	171	C_3H_5-benzene isomer
56	173	C_4-alkyl benzene isomer

(continued)

Table B36 (cont'd)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
57	176	dimethylphenol isomer
57A	178	benzoic acid (tent.) + C_2-alkyl phenol isomer
59	183	trichlorobenzene isomer
60	184	naphthalene
60A	185	benzothiophene
61	186	*n*-dodecane
62	188	$C_{13}H_{26}$ isomer
62A	190	naphthaol isomer (tent.)
63	200	$C_{14}H_{28}$ isomer
64	201	*n*-tridecane
64A	203	β-methylnaphthalene
64B	204	α-methylnaphthalene
66	211	alkyl butyrate isomer (BKG)
67	212	biphenyl
68	215	diphenyl ether
69	220	unsaturated hydrocarbon (tent.)
71	227	*n*-pentadecane
72	229	unknown
73	232	dibenzofuran
76	240	benzophenone
76A	240	$C_{14}H_{10}$ isomer
76B	240	*n*-heptadecane

[a] See Table 31 for protocol.

Table B37. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR FROM NORTH PHILADELPHIA, PA (P3/L3A)[a]

Chromatographic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	52	isobutane
2B	53	C_4H_8 isomer
2C	54	n-butane
3	55	acetaldehyde
3A	58	isopentane
4	59	acetone
4A	62	dichloroethylene isomer
5	63	methylene chloride
7	69	2-methylpentane
8	72	3-methylpentane + butanal
8A	73	methyl ethyl ketone
9	73	hexafluorobenzene (es)
10	74	n-hexane
10A	75	chloroform (traces)
11	76	ethyl acetate
12	78	perfluorotoluene (es)
12A	80	C_6H_{12} isomer
12B	80	1,2-dichloroethane
13	81	1,1,1-trichloroethane
13A	83	$C_5H_{10}O$ aldehyde (traces)
14	84	benzene
14A	85	C_7H_{16} isomer
14B	86	cyclohexane
15	87	2-methylhexane
15A	88	2,3-dimethylpentane
16	89	3-methylhexane
16A	90	pentanal (tent)
17	91	1,2-dichloropropane
17A	91	3-ethylpentane
17B	92	C_7H_{14} isomer
17C	92	trichloroethylene
18	94	n-heptane
18A	95	C_7H_{14} isomer
18B	98	C_8H_{18} isomer
19	99	methylcyclohexane
20	101	acetic acid
20A	103	C_8H_{18} isomer
21	107	toluene
21A	108	C_8H_{18} isomer
22	109	C_8H_{18} isomer
22A	111	C_8H_{16} isomer
23	112	C_8H_{16} isomer
24	115	n-octane
25	116	tetrachloroethylene
25A	121	C_8H_{16} isomer
26	123	C_8H_{16} + C_9H_{20} isomers
26A	124	C_9H_{18} isomer
27	126	ethylbenzene
27A	127	C_9H_{20} isomer
28	128	xylene isomer
28A	128	C_9H_{20} isomer
29	130	C_9H_{20} isomer
30	132	styrene
31	133	o-xylene
31A	134	C_9H_{18} isomer
32	135	n-nonane
33	139	isopropylbenzene
33A	140	$C_{10}H_{22}$ isomer
34	142	$C_{10}H_{22}$ isomer
35	144	benzaldehyde
35A	145	n-propylbenzene
36	146	ethyltoluene isomer
36A	147	1,3,5-trimethylbenzene + benzonitrile (traces)
37	148	phenol
37A	149	$C_{10}H_{22}$ isomer
37B	149	α-methylstyrene
38	149	o-ethyltoluene
38A	150	$C_{10}H_{22}$ isomer
39	151	n-octanal
40	152	1,2,4-trimethylbenzene
40A	153	$C_{10}H_{20}$ isomer
41	154	n-decane
41A	155	dichlorobenzene isomer
42	158	1,2,3-trimethylbenzene
42A	159	$C_{11}H_{24}$ isomer
42B	160	indan
42C	161	$C_{10}H_{16}$ isomer
42D	162	C_4-alkyl benzene isomer
42E	163	C_4-alkyl benzene isomer
43	163	acetophenone
43A	164	cresol isomer
43B	166	$C_{11}H_{22}$ isomer
44	167	C_4-alkyl benzene + $C_{10}H_{16}$ isomer
44A	168	C_4-alkyl benzene isomer
45	169	n-nonanal
45A	170	$C_{11}H_{22}$ isomer
46	171	n-undecane
46A	172	C_4-alkyl benzene isomer
46B	174	C_4-alkyl benzene isomer

(continued)

Table B37 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
47	174	C_4-alkyl benzene isomer
48	176	dimethylphenol isomer
48A	178	C_5-alkyl benzene isomer
49	179	C_2-alkyl phenol isomer
49A	179	C_4H_7-benzne isomer
49B	183	C_5-alkyl benzene isomer
49C	183	C_3-alkyl phenol isomer
49D	185	naphthalene
50	185	n-decanal
50A	186	$C_{12}H_{24}$ isomer
51	187	n-dodecane
51A	191	C_3-alkyl phenol isomer
52	201	n-undecanal
53	202	n-tridecane
53A	203	β-methylnaphthalene
53B	205	α-methylnaphthalene
53C	208	$C_{14}H_{28}$ isomer
53D	209	$C_{13}H_{26}$ isomer
54	211	$C_{15}H_{32}$ isomer (tent)
55	212	alkyl butyrate
55A	213	$C_{14}H_{28}$ isomer
56	215	n-tetradecane
58	224	$C_{16}H_{32}$ isomer
58A	227	$C_{15}H_{30}$ isomer
59	228	n-pentadecane
60	231	unknown
61A	240	$C_{16}H_{32}$ isomer

[a] See Table 31 for protocol.

Table B38. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR IN PHILADELPHIA, PA (P3/L3B)^a

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2A	52	isobutane (tent.)
2B	52	C_4H_8 isomer
2C	53	n-butane
2D	53	acetaldehyde
2E	57	isopentane
3	58	acetone
3A	60	n-pentane (tent.)
4	62	methylene chloride
6	68	2-methylpentane
7	71	3-methylpentane
7A	71	butanal
8	72	hexafluorobenzene (e§)
8A	73	n-hexane
8B	74	chloroform
9	77	perfluorotoluene (e§)
9A	78	methylcyclopentane
9B	79	1,2-dichloroethane
10	80	1,1,1-trichloroethane
11	83	benzene
11A	84	C_7H_{16} isomer + carbon tetrachloride
11B	85	cyclohexane
11C	86	C_7H_{16} isomer
12	86	C_7H_{16} isomer
12A	87	$C_5H_{10}O$ isomer (tent.)
13	88	3-methylhexane
14	89	1,2-dichloropropane
14A	90	C_7H_{16} isomer
14B	91	trichloroethylene
14C	91	C_7H_{14} isomer
14D	92	pentanal (tent.)
15	93	n-heptane
16	98	methylcyclohexane
17	100	acetic acid
18	105	toluene
19	107	C_8H_{18} isomer
20	108	C_8H_{18} isomer
21	111	C_8H_{16} isomer
22	114	n-octane
22A	114	C_8H_{16} isomer
23	115	tetrachloroethylene
23A	121	chlorobenzene (tent.)
24	122	C_9H_{20} isomer
24A	123	C_9H_{18} isomer
25	125	ethylbenzene
25A	126	C_9H_{20} isomer
26	128	xylene isomer
26A	128	C_9H_{20} isomer
27	129	$C_{10}H_{22}$ isomer
27A	130	$C_7H_{14}O$ aldehyde (tent.)
28	131	styrene
29	132	o-xylene
29A	133	C_9H_{18} isomer
29B	134	C_9H_{18} isomer
30	135	n-nonane
31	139	isopropylbenzene
32	142	C_9H_{18} isomer
33	144	benzaldehyde
33A	144	n-propylbenzene
34	146	ethyltoluene (e§)
34A	147	$C_{10}H_{22}$ isomer
35	147	phenol
36	149	α-methylstyrene
37	151	n-octanal
38	152	1,2,4-trimethylbenzene
38A	152	$C_{10}H_{20}$ isomer
39	153	n-decane
39A	154	dichlorobenzene isomer
39B	155	C_4-alkyl benzene isomer
39C	156	C_4-alkyl benzene isomer
39D	156	indan
39E	157	$C_{11}H_{22}$ isomer
40	157	1,2,3-trimethylbenzene
40A	158	$C_{11}H_{24}$ isomer
40B	159	C_3H_5-benzene isomer
40C	160	$C_{11}H_{22}$ isomer
40D	161	C_4-alkyl benzene isomer
40E	162	C_4-alkyl benzene isomer
41	163	acetophenone
41A	163	C_4-alkyl benzene + cresol isomers
41B	165	C_4-alkyl benzene isomer
42	166	2-phenyl-2-propanol (tent.)
42A	167	C_4-alkyl benzene isomer
42B	168	C_4-alkyl benzene isomer
43	169	n-nonanal
43A	169	$C_{11}H_{22}$ isomer
44	171	n-undecane
44A	171	C_4-alkyl benzene isomer
44B	172	C_4-alkyl benzene + $C_{12}H_{26}$ isomers

(continued)

Table B38 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	Chromatographic Peak No.	Elution Temp. (°C)	Compound
45	174	C_4-alkyl benzene isomer	52B	196	$C_{13}H_{28}$ isomer
46	176	C_2-alkyl phenol isomer	53	201	*n*-undecanal
46A	178	$C_{11}H_{22}$ isomer	54	202	*n*-tridecane +
47	179	C_2-alkyl phenol isomer			β-methylnaphthalene
47A	180	C_5-alkyl benzene isomer	54A	204	α-methylnaphthalene
48	181	C_2-alkyl phenol isomer	54B	209	$C_{13}H_{26}$ isomer
49	183	C_3-alkyl phenol isomer	54C	210	$C_{14}H_{28}$ isomer
49A	184	naphthalene	55	211	alkyl butyrate
50	185	*n*-decanal	56	212	alkyl butyrate
50A	186	$C_{12}H_{24}$ isomer	56A	213	biphenyl
51	187	*n*-dodecane	56B	214	C_6-alkyl phenol isomer (tent.)
51A	189	C_3-alkyl phenol isomer	57	216	sat. hydrocarbon
51B	190	C_3-alkyl phenol isomer	58	221	alcohol isomer (tent.)
52	192	unknown	60	229	$C_{15}H_{32}$ isomer
52A	195	$C_{13}H_{26}$ isomer	61	231	alcohol isomer (tent.)

[a] See Table 31 for protocol.

Table B39. VOLATILE ORGANIC VAPORS IDENTIFIED IN AMBIENT AIR FROM PHILADELPHIA, PA (P4/L4B)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2A	51	isobutane
2B	52	C_4H_8 isomer
2C	53	n-butane
2D	53	acetaldehyde
2E	57	isopentane
3	59	acetone
3A	60	n-pentane
3B	61	dichloroethylene
4	62	methylene chloride
5A	65	CS_2 (tent.)
5B	68	butenal or C_5H_{10} isomer
6	69	2-methylpentane
6A	70	methyl isopropyl ketone (tent.)
6B	71	n-butanal
6C	71	3-methylpentane
6D	72	methyl ethyl ketone
7	73	hexafluorobenzene (es)
7A	74	n-hexane
7B	75	chloroform
7C	76	ethyl acetate
8	78	perfluorotoluene (es)
8A	79	methylcyclopentane
9	80	1,2-dichloroethane
9A	81	1,1,1-trichloroethane
10	85	benzene
10A	85	C_7H_{16} isomer
10B	86	carbon tetrachloride
11	86	cyclohexane
11A	87	C_7H_{16} isomer
12	89	3-methylhexane
13	90	1,2-dichloropropane
13A	91	C_7H_{14} isomer
14	92	trichloroethylene + C_7H_{14} isomer
15	94	n-heptane
16	96	C_8H_{16} isomer
17	98	acetic acid
18	99	methylcyclohexane
18A	100	C_8H_{16} isomer
18B	100	C_8H_{18} isomer
19	101	C_8H_{18} isomer
19A	102	C_9H_{20} isomer
20	103	C_8H_{16} isomer
21	104	C_8H_{16} isomer
21A	105	C_8H_{18} isomer
22	106	toluene
23	108	C_8H_{18} isomer
24	109	C_8H_{18} isomer
24A	111	C_8H_{16} isomer
24B	113	$C_6H_{10}O$ isomer
24C	114	C_8H_{16} isomer
25	115	n-octane
26	116	tetrachloroethylene
26A	118	C_8H_{16} isomer
27A	120	C_9H_{20} isomer
27B	120	C_9H_{18} isomer
28	121	C_9H_{18} isomer
29	123	chlorobenzene
30	124	C_9H_{18} isomer
30A	125	C_9H_{18} isomer
31	126	ethylbenzene
31A	127	C_9H_{18} isomer
32	128	xylene
33	130	C_9H_{20} isomer
33A	131	$C_7H_{14}O$ isomer
34	131	styrene
35	133	o-xylene
35A	133	$C_{10}H_{22}$ isomer
35B	134	C_9H_{18} isomer
36	135	n-nonane
37	139	isopropylbenzene
38	140	$C_{10}H_{22}$ isomer
38A	142	$C_{10}H_{22}$ isomer
39	142	C_9H_{18} isomer
40	144	benzaldehyde
41	144	n-propylbenzene
41A	145	$C_{10}H_{20}$ isomer
42	146	ethyltoluene
42A	147	$C_{10}H_{22}$ isomer
43	147	1,3,5-trimethylbenzene + benzonitrile
43A	147	phenol
43B	148	$C_{10}H_{22}$ isomer
43C	149	$C_{10}H_{22}$ isomer
44	149	o-ethyltoluene + $C_8H_{16}O$ isomer (tent.)
44A	151	$C_{10}H_{20}$ isomer
45	151	n-octanal
45A	152	$C_{10}H_{20}$ isomer
46	152	1,2,4-trimethylbenzene
46A	153	$C_{10}H_{20}$ isomer

(continued)

Table B39 (cont'd)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
47	154	*n*-decane
48	155	dichlorobenzene
48A	155	C_4-alkyl benzene isomer
48B	156	$C_{11}H_{22}$ isomer
48C	157	C_4-alkyl benzene isomer
49	157	1,2,3-trimethylbenzene
49A	158	C_4-alkyl benzene isomer
50	158	$C_{11}H_{24}$ isomer
51	159	dichlorobenzene + $C_{11}H_{24}$ isomers
51A	160	indan
51B	161	$C_{10}H_{20}$ isomer
52	162	C_4-alkyl benzene isomer
53	163	acetophenone
53A	163	C_4-alkyl benzene isomer
53B	164	cresol isomer (tent.)
54	165	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
54A	167	C_4-alkyl benzene isomer
54B	168	C_3H_5-benzene
54C	168	C_4-alkyl benzene isomer
55	169	*n*-nonanal
55A	170	$C_{11}H_{22}$ isomer
56	171	*n*-undecane
57	172	methylindene
57A	174	C_4-alkyl benzene isomer
58	175	C_4-alkyl benzene isomer
58A	175	unsat. hydrocarbon
59	176	C_2-alkyl phenol
59A	179	C_2-alkyl phenol
59B	180	C_4H_7-benzene
60	180	C_5-alkyl benzene + $C_{13}H_{28}$ isomers
60A	184	$C_{10}H_{20}O$ isomer (tent.)
60B	184	$C_{12}H_{24}$ isomer
61	185	naphthalene + *n*-decanal
61A	186	$C_{12}H_{24}$ isomer
62	187	*n*-dodecane
63	201	unsat. hydrocarbon
64	202	*n*-tridecane
64A	202	β-methylnaphthalene
64B	205	α-methylnaphthalene
65	208	tetraisobutylene (tent.)
66	212	alkyl butyrate
66A	213	biphenyl
66B	214	$C_{14}H_{28}$ isomer
67	216	*n*-tetradecane + diphenyl ether
67A	220	C_2-alkyl naphthalene
68	221	unsat. hydrocarbon
68A	228	$C_{15}H_{30}$ isomer
69	229	*n*-pentadecane
70	231	unknown

[a] See Table 31 for protocol.

Table B40. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR FROM MARCUS HOOK, PA (P5/L5A)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO_2
2	51	isobutane
3	53	C_4H_8 isomer
3A	53	*n*-butane
4	54	C_4H_8 isomer
5	55	C_4H_8 isomer
5A	57	C_5H_{10} isomer
5B	58	C_5H_{10} isomer
6	59	isopentane
7	60	C_5H_{10} isomer
8	61	*n*-pentane
8A	61	C_5H_{10} isomer
9	62	C_5H_{10} isomer
10	63	C_5H_{10} isomer
11	64	C_5H_{10} isomer
11A	68	cyclopentane
12	69	C_6H_{12} isomer
12A	70	C_5H_{10} isomer
13	70	2-methylpentane
13A	71	C_6H_{12} isomer
14	73	3-methylpentane
15	73	C_6H_{12} isomer
16	74	hexafluorobenzene (eS)
17	75	*n*-hexane
18	76	C_6H_{12} isomer
19	77	C_6H_{12} + C_6H_{10} isomers
20	78	C_6H_{12} isomer
20A	78	C_6H_{10} isomer
21	79	C_6H_{12} isomer
22	80	perfluorotoluene (eS)
23	81	C_6H_{12} isomer
24	83	1,1,1-trichloroethane
24A	84	C_7H_{14} isomer
25	85	C_6H_{10} isomer
26	86	benzene
26A	86	C_7H_{16} isomer
26B	87	C_7H_{14} isomer
26C	88	cyclohexane
27	89	2-methylhexane
27A	90	2,3-dimethylpentane
28	91	3-methylhexane
28A	91	C_7H_{14} isomer
29	93	C_7H_{14} isomer
29A	94	C_8H_{18} isomer
29B	95	C_7H_{14} isomer
30	95	*n*-heptane
30A	96	C_7H_{14} isomer
30B	96	C_7H_{12} isomer
31	97	C_7H_{14} isomer
32	98	C_7H_{12} + C_7H_{14} isomers
32A	100	C_7H_{12} isomer
33	101	methylcyclohexane
34	102	C_8H_{18} isomer
34A	102	acetic acid
35	103	C_8H_{18} isomer
35A	104	C_7H_{12} isomer
36	104	C_8H_{16} isomer
36A	106	C_8H_{14} isomer
36B	106	C_8H_{16} isomer
36C	106	C_7H_{12} isomer
37	107	C_8H_{18} isomer
37A	107	C_8H_{16} isomer
38	108	toluene
39	110	C_8H_{18} isomer
40	111	C_8H_{18} isomer
41	113	C_8H_{16} isomer
42	113	C_8H_{16} isomer
43	115	C_8H_{16} isomer
44	115	C_8H_{16} isomer
45	117	*n*-octane
45A	117	C_8H_{16} isomer
45B	118	tetrachloroethylene
46	118	C_8H_{16} isomer
46A	120	C_9H_{18} isomer
47	120	C_9H_{20} isomer
48	122	C_9H_{20} isomer
48A	122	C_9H_{16} isomer
49	123	C_9H_{20} isomer
49A	124	C_8H_{16} isomer
50	124	C_9H_{20} isomer
51	126	C_9H_{18} isomer
52	128	ethylbenzene
53	129	C_9H_{18} isomer
54	130	xylene isomer
54A	130	C_9H_{20} isomer
55	131	C_9H_{20} isomer
55A	133	C_9H_{18} isomer
56	134	C_9H_{18} isomer
57	135	*o*-xylene
58	136	C_9H_{18} isomer
59	137	*n*-nonane
59A	138	$C_{10}H_{20}$ isomer

(continued)

Table B40 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
60	140	C_9H_{18} isomer
61	141	isopropylbenzene + $C_{10}H_{22}$ isomer
62	142	C_9H_{16} + $C_{10}H_{22}$ isomers
63	144	C_9H_{18} + $C_{10}H_{22}$ isomers
64	146	benzaldehyde
64A	146	$C_{10}H_{20}$ isomer
65	146	*n*-propylbenzene
66	148	ethyltoluene isomer
66A	149	$C_{10}H_{22}$ isomer
67	149	1,3,5-trimethylbenzene + $C_{10}H_{22}$ isomer
67A	150	$C_{11}H_{24}$ isomer
68	151	$C_{10}H_{22}$ isomer
69	151	*o*-ethyltoluene
70	152	$C_{10}H_{22}$ isomer
71	153	$C_{10}H_{20}$ isomer
71A	154	$C_{10}H_{20}$ isomer
72	154	1,2,4-trimethylbenzene
72A	155	$C_{10}H_{20}$ isomer
73	156	*n*-decane
74	157	$C_{10}H_{20}$ isomer
74A	157	C_4-alkyl benzene isomer
75	159	C_4-alkyl benzene + $C_{11}H_{24}$ isomers
76	159	1,2,3-trimethylbenzene
77	160	$C_{11}H_{24}$ isomer
78	161	$C_{11}H_{24}$ isomer
78A	162	indan
79	163	$C_{16}H_{20}$ isomer
79A	163	C_4-alkyl benzene isomer
80	164	C_4-alkyl benzene isomer
81	165	acetophenone + C_4-alkyl benzene isomer
82	166	$C_{11}H_{22}$ isomer
83	167	$C_{11}H_{24}$ + C_4-alkyl benzene isomers
83A	168	$C_{10}H_{18}$ isomer
84	168	$C_{11}H_{24}$ isomer
84A	169	C_4-alkyl benzene isomer
85	170	C_4-alkyl benzene isomer
85A	171	C_4H_7-benzene isomer
86	171	$C_{11}H_{22}$ isomer
87	173	*n*-undecane
87A	173	C_5-alkyl benzene isomer
87B	174	C_4-alkyl benzene isomer
88	174	$C_{11}H_{22}$ isomer
89	176	C_4-alkyl benzene isomer
90	178	$C_{12}H_{26}$ + C_2-alkyl phenol isomers
90A	178	C_5-alkyl benzene isomer
90B	180	$C_{11}H_{22}$ isomer
91	180	$C_{11}H_{20}$ isomer
91A	181	C_5-alkyl benzene + C_2-alkyl phenol isomers
91B	181	C_4H_7-benzene isomer
92	182	$C_{12}H_{26}$ isomer
92A	183	C_5-alkyl benzene isomer
93	183	C_5-alkyl benzene + $C_{12}H_{26}$ isomers
94	185	C_5-alkyl benzene isomer
95	187	naphthalene
95A	187	*n*-decanal (tent.)
95B	188	$C_{12}H_{24}$ isomer
96	189	*n*-dodecane
96A	190	C_6-alkyl benzene isomer (tent.)
97	191	$C_{13}H_{28}$ isomer
97A	192	C_6-alkyl benzene isomer
97B	195	$C_{13}H_{26}$ isomer
97C	196	$C_{12}H_{24}$ isomer
98	197	C_5H_9-benzene + $C_{13}H_{26}$ isomers
99	199	$C_{13}H_{28}$ isomer (tent.)
100	200	$C_{14}H_{30}$ isomer
100A	201	$C_{14}H_{28}$ isomer
101	203	*n*-tridecane
101A	204	β-methylnaphthalene
101B	205	$C_{14}H_{28}$ isomer
102	206	α-methylnaphthalene
103	211	$C_{13}H_{26}$ isomer
104	212	$C_{14}H_{30}$ isomer
105	214	alkyl butyrate
106	215	$C_{15}H_{32}$ isomer
106A	215	$C_{14}H_{28}$ isomer
107	217	*n*-tetradecane
107A	218	C_2-alkyl naphthalene
107B	219	$C_{14}H_{28}$ isomer
108	220	C_2-alkyl naphthalene
109	222	C_2-alkyl naphthalene + $C_{15}H_{30}$ isomers
110	226	$C_{16}H_{34}$ isomer
110A	228	$C_{15}H_{30}$ isomer
111	230	*n*-pentadecane

(continued)

Table B40 (cont'd)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
112	232	unknown
116	240	sat. hydrocarbon
117	240	$C_{15}H_{30}O$ isomer (tent.)
118	240	*n*-heptadecane
119	240	sat. hydrocarbon

[a] See Table 31 for protocol.

Table B41. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR FROM LOGAN TOWNSHIP, NJ (P8/L8A)[a]

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO_2
2A	53	C_4H_8 isomer
3	54	acetaldehyde
3A	58	isopentane
4	60	acetone
4A	61	n-pentane (tent.)
4B	62	diethyl ether (tent.)
4C	62	dichloroethylene
5	63	methylene chloride
6A	68	butenal isomer
7	69	2-methylpentane
7A	71	butanal
8	71	3-methylpentane
9	73	hexafluorobenzene (e[illegible])
9A	75	n-hexane
9B	76	chloroform
9C	77	ethyl acetate
10	79	perfluorotoluene (e[illegible])
10A	80	methylcyclopentane
11	82	1,1,1-trichloroethane
12	85	benzene
12A	85	C_7H_{16} isomer
12B	86	carbon tetrachloride (tent.)
12C	87	cyclohexane
13	87	2-methylhexane
13A	88	2,3-dimethylpentnae
14	89	3-methylhexane
14A	90	n-pentanal
14B	91	C_7H_{14} isomer
15	91	3-ethylpentane
16	92	C_7H_{14} isomer + trichloroethylene (tent.)
17	94	n-heptane
18	99	acetic acid
18A	100	methylcyclohexane
19	101	C_8H_{18} isomer
20	103	C_8H_{18} isomer
20A	106	C_8H_{16} isomer
21	107	toluene
21A	109	C_8H_{18} isomer
21B	110	C_8H_{18} isomer
22	112	n-hexanal
22A	113	C_8H_{16} isomer
23	115	n-octane
24	116	tetrachloroethylene
24A	123	chlorobenzene
25	127	ethylbenzene
25A	127	C_9H_{18} isomer
26	128	xylene isomer
26A	129	C_9H_{18} isomer
26B	131	C_9H_{20} isomer
26C	132	styrene
27	133	n-heptanal
27A	133	o-xylene
28	136	n-nonane
28A	138	$C_{10}H_{22}$ isomer
28B	139	C_9H_{18} isomer
29	145	benzaldehyde
29A	146	n-propylbenzene
30	147	ethyltoluene + $C_{10}H_{22}$ isomers
31	149	phenol + $C_{11}H_{24}$ isomer
31A	149	C_9H_{18} isomer
31B	150	C_3-alkyl benzene isomer
32	152	n-octanal
32A	153	1,2,4-trimethylbenzene
33	154	n-decane
33A	155	dichlorobenzene isomer (tent.)
33B	158	1,2,3-trimethylbenzene
34	160	$C_{11}H_{24}$ isomer
34A	163	C_4-alkyl benzene isomer
35	164	acetophenone
35A	165	C_4-alkyl benzene isomer
35B	165	cresol isomer
35C	166	C_4-alkyl benzene isomer
35D	169	$C_{11}H_{22}$ isomer
36	170	n-nonanal
37	172	n-undecane
37A	175	C_4-alkyl benzene isomer
38	177	C_2-alkyl phenol isomer
39	181	C_2-alkyl phenol isomer
40A	185	naphthalene
41	186	n-decanal
41A	187	$C_{12}H_{24}$ isomer
42	188	n-dodecane
42A	190	C_3-alkyl phenol isomer
43	193	unknown
44	201	$C_{11}H_{22}O$ isomer
45	202	n-tridecane
45A	203	β-methylnaphthalene
46	209	unsat. hydrocarbon (tent.)
47	211	sat. hydrocarbon (tent.)
48	213	alkyl butyrate

(continued)

Table B41 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound
48A	214	biphenyl (traces)
49	216	n-tetradecane
50	221	unknown
51	223	unsat. hydrocarbon
52	225	sat. hydrocarbon
53	228	$C_{15}H_{30}$ isomer
54	229	n-pentadecane
55	231	unknown

[a] See Table 31 for protocol.